projection on (010) 1·59$_4$ Å) probably due to the combined effect of ring strain and steric repulsion of the non-bonded oxygen atoms. It is worthy of note that in pyracene a value of 1·59 ± 0·03 Å was found for this distance, although the authors did not consider it to be significantly stretched. The short *peri*-bond length of 1·48 ± 0·01$_0$ Å is unexpected, and its significance cannot be judged until further data for *cis*-1,2-substituted acenaphthenes are available. It may be pointed out, however, that a similar bond-shortening effect has been observed in *cis*-1,2-dichlorobenzocyclobutene, which has an average *peri*-bond distance of 1·45 ± 0·01 Å (Hardgrove, 1959; Hardgrove & Templeton, 1961). The C–O bond has a length of 1·45 ± 0·01$_0$ Å which is typical of aliphatic alcohols (*Tables of Interatomic Distances and Configurations in Ions and Molecules*, 1958). In the naphthalene ring the C(3)–C(4) and C(4)–C(5) bonds are respectively the longest and the shortest, in agreement with the bond-length variations observed in all acenaphthene derivatives so far examined.

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References

CRUICKSHANK, D. W. J. (1949). *Acta Cryst.* **2**, 154.
CSIZMADIA, I. G. & HAYWARD, L. D. (1962). In preparation.
EHRLICH, H. W. W. (1957). *Acta Cryst.* **10**, 699.
HARDGROVE, G. L. (1959). Thesis, University of California, Berkeley.
HARDGROVE, G. L. & TEMPLETON, D. H. (1961). Programs and Abstracts, Amer. Cryst. Assoc. Annual Meeting.
I.U.P.A.C. 1957 Rules. *Nomenclature of Organic Chemistry*. London: Butterworths.
KLYNE, W. & PRELOG, V. (1960). *Experientia*, **16**, 521.
MAK, T. C. W. & TROTTER, J. (1963). *Acta Cryst.* **16**, 811.
MORICONI, E. J., O'CONNOR, W. F., KUHN, L. P., KENEALLY, E. A. & WALLENBERGER, F. T. (1959). *J. Amer. Chem. Soc.* **81**, 6472.
PAULING, L. (1960). *Nature of the Chemical Bond*, p. 453. Ithaca, New York: Cornell University Press.
PIMENTEL, G. C. & MCCLELLAND, A. L. (1960). *The Hydrogen Bond*, p. 271. San Francisco: Freeman.
ROSSMANN, M. G. & SHEARER, H. M. M. (1958). *Acta Cryst.* **11**, 829.
SAGEL, K. (1958). *Tabellen zur Röntgenstrukturanalyse*. Berlin: Springer.
SIMMONS, G. L. & LINGAFELTER, E. C. (1961). *Acta Cryst.* **14**, 872.
Tables of Interatomic Distances and Configurations in Ions and Molecules (1958). Special Publ. No. 11. London: The Chemical Society.

Acta Cryst. (1963). **16**, 1037

The Crystal Structure of $LiCuCl_3.2H_2O$*

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$LiCuCl_3.2H_2O$ forms garnet-red, monoclinic crystals, $a = 6{\cdot}078$, $b = 11{\cdot}145$, $c = 9{\cdot}145$ Å (all ±0·003), $\beta = 108°\ 50'$, space group $P2_1/c$, $Z = 4$. The structure contains planar $[Cu_2Cl_6]^{2-}$ ions joined by longer Cu · · · Cl links to form chains. Half of the water molecules are coordinated to copper.

A final refinement using the Levy–Busing anisotropic temperature factor treatment and least-squares program achieved a discrepancy index, R, of 10·5% for our visually determined intensities. Standard deviations as determined from least squares are about 0·007 Å for oxygen parameters, less for others, while important interatomic distances have been determined with standard deviations of ~0·0025 Å.

The structure has very interesting magnetic properties, reported elsewhere (Vossos, Jennings & Rundle, 1960). Because of this, a neutron diffraction study is under way at Brookhaven by S. C. Abrahams.

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

Introduction

The garnet-red crystals of $LiCuCl_3.2H_2O$ were first reported by Chassevant (1891), but the composition was settled by Meyerhoffer (1892). Attempts to

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interpret the formula and discuss the color in terms of complex ions by Donnan (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 $[Cu_2Cl_6]^{2-}$ ion, complete structural work was undertaken. Simultaneously this ion was found in $KCuCl_3$ (Dwiggins, 1958). A brief announcement of structural and magnetic properties has been published (Vossos, Jennings & Rundle, 1960).

Preparation and properties

$LiCuCl_3.2H_2O$ was prepared by the method of Getman (1922). The prismatic, monoclinic crystals are elongated along what we have chosen as the a axis. The dominant face is (011). The garnet-red crystals are strongly pleochroic. The crystal density, determined by flotation, is 2·36 g.cm^{-3}. 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 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 $2/m$ (C_{2h}) Laue symmetry. Lattice constants determined by the back reflection Weissenberg technique (Buerger, 1942) were: $a=6{\cdot}078$, $b=11{\cdot}145$, $c=9{\cdot}145\pm0{\cdot}003$ Å, $\beta=108°\ 50'$. The X-ray density for $Z=4$ is 2·39 g.cm^{-3}, 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 Mo $K\alpha$ 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 position and a clue

Table 1. *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(1)	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(2)	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(3)	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(1)	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(2)	x	0·6466	0·0019	0·64661	0·00107
	y	0·3954	0·0009	0·29556	0·00065
	z	0·0350	0·0011	0·03522	0·00081

* Isotropic thermal parameters.
† Anisotropic thermal parameters.

Table 2. *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 3. *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(1)	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(2)	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(3)	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(1)	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(2)	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 4. *List of observed and calculated structure factors*

The calculated structure factors are scaled to the observed data as given in Table 2. Columns are from left to right, running index l, $|F|_o$ and F_c

0 0

2	4.9	3.91
4	24.9	-30.26
6	7.4	- 7.47
8	3.4	2.62
10	9.7	9.33
12	3.5	- 1.86
14	3.9	- 3.90

0 1

2	8.2	- 7.96
3	6.2	- 7.50
4	5.0	5.26
5	27.9	-34.17
6	3.0	3.44
7	2.4	2.32
8	4.2	- 3.67
9	13.4	12.47
10	3.9	- 3.31

0 2

2	3.4	3.78
3	4.4	3.47
4	17.5	-17.94
5	10.3	8.77
6	4.6	- 5.63
7	9.7	8.86
8	6.4	5.90
9	7.1	- 6.82
10	4.9	5.10
11	4.5	- 4.32

0 3

1	9.1	9.64
2	10.5	-10.80
3	10.1	-10.92
4	7.6	7.81
5	2.1	- 1.37
8	4.8	- 4.62
9	5.8	4.79
10	3.1	- 2.77
13	4.6	- 4.13

0 4

0	20.1	-20.37
1	6.7	6.10
2	2.5	3.08
4	6.7	- 6.51
6	4.0	- 4.54
7	4.1	4.57
8	11.1	10.63

0 5

1	12.5	12.63
3	11.5	-12.47
5	3.6	3.13
6	3.4	- 2.96
7	2.6	2.60
8	2.8	1.83
9	3.0	2.37
13	5.7	- 4.98

0 6

0	8.9	8.85
1	4.7	- 3.82
2	3.3	3.31
3	5.7	- 5.89
4	13.3	-13.27
5	3.9	- 4.41
6	7.2	- 7.35
7	3.5	- 2.66
8	9.2	9.48
9	4.4	4.24

0 7

1	18.7	19.68
3	9.7	- 9.33
4	9.4	- 7.75
5	15.4	-16.44
6	4.3	4.04
8	5.4	4.77
9	6.8	6.32

0 8

0	29.5	32.35
1	13.1	-11.94
2	3.9	3.58
3	5.8	- 5.55
4	16.0	-16.61
5	2.2	3.77
6	6.9	- 7.40
8	4.5	3.28
10	5.9	6.12

0 9

1	12.5	11.47
2	3.3	- 4.15
3	2.8	- 2.90
4	2.6	- 2.19
5	16.6	-17.95
6	8.9	9.24
9	8.1	7.24
10	5.7	- 5.53

0 10

0	16.4	16.26
1	3.9	- 4.77
4	6.8	- 7.11
5	7.5	6.78
7	3.2	3.95
9	3.8	- 3.79
10	3.4	4.01

0 11

2	4.5	- 4.76
4	3.7	4.01
5	4.2	- 3.94
6	3.5	2.40
9	4.6	3.94
10	3.7	- 3.07

0 12

1	3.7	3.49
7	4.4	3.90

0 13

2	4.3	- 3.75
3	3.2	- 2.72

0 14

4	4.7	- 3.96
8	4.9	4.09

0 15

1	7.0	6.64
2	3.4	- 3.78
3	4.8	- 4.16
4	3.6	- 2.37
5	4.1	- 3.25

0 16

0	6.0	5.77
1	5.6	- 4.94
4	4.7	- 4.56

0 17

6	5.5	4.70

1 0

2	11.2	10.14
4	5.1	4.09
6	15.5	-15.41
8	7.3	- 7.41
- 8	2.2	- 1.34
-10	7.0	- 6.92

1 1

2	23.2	26.08
3	12.4	14.33
- 3	4.3	- 3.74
4	4.3	3.47
- 4	9.7	- 9.55
5	16.1	-19.07
- 5	4.9	4.15
6	8.7	- 8.21
- 6	5.0	- 4.38
7	8.6	- 8.96
- 7	6.3	5.41
- 8	7.5	6.72
9	2.0	1.08
- 9	1.9	1.79
-10	2.6	- 2.25
-11	5.3	- 4.62
-13	2.5	- .87
-15	2.8	2.79

1 2

2	16.5	17.03
3	4.6	- 3.07
- 3	24.7	-33.03
- 4	14.7	-18.97
5	1.5	- 1.57
- 5	5.6	4.73
6	13.0	-12.38
- 6	7.6	8.90
7	9.1	- 9.07
- 7	2.2	1.95
8	1.9	- 1.52
- 8	9.6	9.41
9	3.3	- 3.01
- 9	1.9	1.68
10	6.6	6.27
-10	2.5	- 2.75
11	3.8	3.84
-11	5.4	4.85
-12	4.3	- 3.70
-15	2.3	.85

1 3

1	18.0	22.80
- 1	5.7	- 4.85
2	19.1	24.20
- 2	5.2	3.96
3	4.3	5.19
- 3	28.1	-32.87
4	5.4	4.30
- 4	10.2	-11.40
5	6.1	- 6.55
- 5	5.8	- 5.66
6	9.3	- 8.98
- 6	7.2	- 7.30
7	4.7	- 4.61
- 7	16.0	16.06
8	9.2	8.47
9	4.3	4.47
- 9	7.3	7.64
-10	2.1	- 1.95
11	2.7	2.45
-11	5.4	- 5.04
-13	5.8	- 4.82
-14	2.7	1.06

1 4

0	8.4	9.06
1	5.9	3.36
- 1	2.4	3.21
2	20.2	25.53
- 2	16.7	-19.80
3	8.9	- 8.48
- 3	5.7	- 4.82
4	6.4	- 6.59
- 4	12.9	-15.51
6	8.6	- 7.99
- 6	7.5	8.17
8	3.4	3.46
- 8	18.1	18.87
9	2.4	- 1.71
-10	3.2	2.46
11	2.4	.79
-11	3.1	2.64
-12	9.5	- 9.00
-14	3.3	- 2.07

1 5

0	1.7	1.81
1	11.0	11.39
- 1	2.1	- 2.64
2	16.4	-16.62
- 2	10.0	9.23
3	7.6	7.58
- 3	24.3	-32.52
4	2.5	- 3.07
- 4	2.5	2.51
- 5	6.3	- 6.41
6	6.3	5.78
- 6	2.5	- 2.15
7	7.3	- 7.03
- 7	16.4	17.84
8	2.7	2.82
- 9	3.6	3.93
-10	2.7	2.54
11	3.0	2.77
-11	4.6	- 4.17
-13	4.0	- 3.82

1 6

0	4.6	4.83
1	12.3	-12.66
- 1	5.0	5.81
2	18.0	21.42
- 2	16.3	-17.27
3	5.9	- 5.83
- 3	15.9	18.84
4	4.4	- 3.82
	1.5	- 1.88
- 5	5.2	- 5.85
6	8.7	- 8.37
- 6	5.8	5.39
7	10.0	9.99
- 7	2.5	- 1.76
- 8	8.4	8.11
9	2.9	2.89
11	3.6	- 3.67
-11	3.1	- 2.66
-12	6.2	- 6.-1

1 7

0	4.8	4.68
1	8.4	7.97
- 1	3.1	- 2.59
2	16.5	-17.66
- 2	2.0	1.08
3	10.7	10.83
- 3	9.7	- 9.72
4	7.5	- 8.46
- 4	4.0	4.26
5	6.2	- 6.17
- 6	8.3	8.53
7	2.5	2.52
- 8	9.7	- 9.99
10	7.8	7.10
-11	4.5	- 4.35
- 9	3.1	- 2.51
6	2.4	.19
- 6	3.3	3.14
- 7	4.8	4.89
- 8	3.6	- 2.95

1 8

0	6.0	5.45
- 1	4.4	4.60
2	9.9	9.20
- 2	8.3	- 7.86
3	2.3	2.05
- 3	4.3	4.05
- 4	3.6	- 3.22
5	3.3	- 2.74
- 5	5.3	- 6.14
6	10.3	- 9.95
- 6	4.4	3.90
7	3.5	2.79
- 7	4.3	- 4.67
8	2.1	- 1.30
- 8	3.5	4.20
10	6.1	6.00
-10	3.6	- 3.35
11	3.3	- 2.88
-11	3.4	- 3.05

1 9

0	6.5	7.07
1	13.0	13.34
- 1	3.2	- 2.97
2	4.8	4.85
- 2	4.8	- 4.98
3	5.0	4.61
- 3	1.8	- 1.5
- 5	4.4	- 5.00
- 6	6.3	- 5.77
7	11.1	-10.75
- 7	1.9	1.32
8	4.9	- 4.32
- 8	3.0	2.20
- 9	2.3	1.75
-11	3.1	- 2.84

0 10

0	7.8	7.24
- 1	10.0	8.98
2	2.9	3.26
- 2	2.8	2.67
3	4.0	- 3.43
- 3	10.9	- 9.87
6	13.4	-13.10
7	2.3	- 2.88
- 5	4.0	- 4.42
6	6.8	- 6.73
- 6	4.3	4.14
- 2	3.3	- 3.39
3	4.4	4.10
- 3	3.4	3.31
4	5.8	5.54
6	2.5	- 2.29

1 11

0	4.1	4.20
1	11.7	11.87
2	7.6	6.82
- 1	3.3	- 2.93
- 2	2.6	2.11
- 3	8.1	- 8.08
- 4	8.2	- 7.88
5	7.1	- 6.43
- 5	2.1	- 2.01
6	3.8	- 3.62
- 6	4.7	- 4.62
- 7	4.4	4.34
- 8	5.6	4.97
- 9	6.9	6.80
-11	2.6	- 2.59
-13	3.6	- 3.43

1 12

0	4.1	3.59
1	3.0	3.20
- 1	3.9	4.21
2	5.3	5.15
- 2	6.9	- 6.28
3	6.6	- 6.76
- 3	3.8	- 3.55
- 4	9.8	- 9.62
- 5	2.2	- 2.12
- 6	2.9	- 2.45
- 7	3.7	3.65
- 8	2.3	- 1.71
8	8.1	8.23
- 9	3.2	3.31
-11	3.3	2.90
-12	3.6	- 3.07
-13	2.9	- 2.06

1 13

1	3.9	3.37
- 1	2.9	- 2.43
2	4.6	- 4.41
- 2	8.6	7.91
3	4.0	4.01
- 3	9.3	- 9.28
- 5	2.3	- 1.33
- 6	4.9	- 4.68
7	2.5	- 2.42
- 7	5.8	6.34
- 8	3.4	3.53
- 8	2.5	2.03
- 9	2.6	2.58

1 14

1	3.1	- 2.85
- 1	3.8	3.89
2	7.7	7.33
- 2	6.7	- 6.32
- 3	7.9	- 7.39
3	3.7	3.34
- 4	2.5	- 2.05
7	5.3	4.89

1 15

1	2.4	- .15
2	5.2	- 5.15
- 2	3.3	2.78
3	4.6	4.26
- 3	3.8	- 3.72
4	3.3	- 3.29
6	2.6	2.30

Table 4 (*cont.*)

1 15			2 2			2 5			2 7			2 11			3 0		
7	4.8	- 4.88	5	6.5	6.86	2	3.6	2.91	-12	3.0	- 2.57	5	4.9	4.85	2	6.6	4.68
- 7	3.3	3.17	- 5	4.5	- 3.71	- 2	11.7	-11.01	-15	2.8	2.61	- 5	10.1	9.95	4	10.0	10.14
8	2.7	2.79	6	5.9	- 6.25	3	24.9	25.28	2 8			6	2.3	- 2.75	6	4.0	4.30
			- 6	15.1	15.09	- 3	4.4	- 4.34	0	3.7	- 3.40	- 6	6.6	- 6.39	- 6	5.2	4.55
1 16			7	6.0	- 6.29	4	3.8	- 2.84	1	2.2	2.50	7	2.9	- 2.66	- 8	12.6	-11.18
- 1	2.5	2.02	- 7	6.8	- 7.12	- 4	2.6	- 2.49	- 1	6.7	7.00	- 7	2.0	1.53	-10	13.6	-13.53
2	4.2	4.22	8	5.9	- 5.96	5	2.5	2.93	2	3.3	2.90	8	2.2	1.35	-12	2.1	.56
- 2	3.3	- 2.08	8	2.1	1.49	- 5	8.6	8.47	4	2.8	- 2.11	9	4.1	- 4.21	-14	6.7	7.27
6	3.3	- 2.97	9	2.2	- 2.25	6	1.9	- 1.78	- 4	3.4	3.18	- 9	4.0	- 3.67	3 1		
			- 9	2.9	- 2.88	- 6	9.3	8.81	5	3.7	- 3.93	-10	2.5	2.00	1	30.2	-24.54
1 17			-10	9.2	- 8.60	7	10.0	-11.09	- 5	1.6	- .98	-13	2.5	.72	2	5.2	5.13
0	3.4	3.1	-11	8.2	7.46	- 7	13.7	14.89	6	4.5	- 4.28	2 12			3	2.0	- 1.42
1	3.2	2.29	12	2.6	2.25	8	2.8	2.19	- 6	5.2	4.56	0	8.1	- 8.12	4	7.4	- 6.29
- 2	2.9	- 2.07	-14	3.7	3.47	- 8	4.1	4.44	7	3.5	3.63	1	4.3	4.93	5	12.9	14.06
4	2.7	- 2.66	-15	2.7	- 2.02	9	4.2	- 4.25	- 8	2.5	2.39	- 1	6.9	6.89	- 5	21.9	28.23
						- 9	2.2	- 1.93	- 9	4.8	4.34	2	6.3	5.88	6	4.6	- 4.63
1 18			2 3			10	2.8	2.79	-10	6.6	- 6.42	- 2	9.3	- 9.50	- 6	2.9	3.00
0	2.7	2.32	0	5.1	- 4.59	-10	2.8	- 2.04	-11	2.9	- 2.61	- 3	5.9	- 6.44	7	3.0	- 3.33
1	2.7	2.10	2	7.3	6.68	-11	6.3	- 6.40	-12	3.1	- 2.21	4	9.9	10.46	- 7	1.9	- 2.19
			- 2	4.7	3.82	12	2.4	- 1.36	-14	3.1	2.76	5	2.1	- 2.52	8	1.9	- .82
1 19			3	21.2	25.67	-12	4.1	- 4.11	2 9			- 5	2.6	- 2.22	- 8	2.4	- 2.16
0	2.8	2.72	- 3	6.5	- 6.50	-13	3.4	3.64	0			- 6	7.3	7.11	9	3.6	- 3.30
1	3.6	3.04	4	7.3	- 7.35	2 6			1	5.2	4.70	7	3.0	- 2.86	- 9	17.6	-18.53
- 4	3.5	- 2.58	5	4.7	5.03	0	3.1	- 3.36	- 1	4.2	3.99	- 7	4.7	4.54	-13	5.6	5.32
- 5	3.2	- 1.07	- 5	13.7	15.29	1	1.9	2.61	2	4.3	- 4.37	8	5.1	- 5.13	3 2		
			6	2.8	- 2.41	- 1	12.8	-13.37	- 2	2.1	- 1.44	9	3.3	2.51	1	10.2	8.00
1 20			- 6	14.2	-15.29	2	10.6	11.22	- 3	5.7	5.72	-10	3.3	- 2.73	2	2.7	- 3.11
- 4	2.9	- 3.07	7	9.5	- 9.91	- 2	17.6	-20.77	- 4	4.2	- 3.62	2 13			3	3.7	4.02
			- 7	10.9	11.48	3	3.0	2.49	5	4.4	- 5.12				4	8.9	9.37
1 21			8	2.6	2.39	- 3	5.2	- 5.85	- 5	2.0	1.32	- 1	5.9	- 8.36	- 4	17.8	19.28
- 3	1.0	1.31	9	5.3	- 5.61	4	7.1	7.15	6	9.8	9.65	2	5.3	5.16	5	8.7	- 8.42
			- 9	4.7	- 4.59	- 4	3.6	3.62	- 6	1.9	- 2.11	- 2	6.1	- 6.17	- 5	11.4	-11.04
2 0			10	2.7	- 2.36	5	6.4	- 7.45	7	2.0	- 1.03	3	8.3	8.63	6	4.6	5.11
2	4.7	5.41	-10	5.1	4.63	- 5	1.4	1.64	- 9	5.6	- 5.24	- 3	3.7	- 3.59	- 6	2.8	2.84
4	2.4	- 1.70	11	2.2	1.80	- 6	11.2	11.36	11	3.1	3.11	4	5.3	- 5.04	7	4.3	- 4.38
6	9.2	-10.78	-11	5.8	- 5.62	7	3.6	4.22	-11	2.9	- 2.75	- 4	2.0	- 1.76	- 7	3.0	2.58
- 8	8.4	7.58	12	2.6	2.12	- 7	9.9	10.03	-12	2.3	1.55	5	2.8	2.55	8	1.9	- 2.35
10	2.8	2.07	-12	2.1	.76	8	6.7	- 6.34	-15	3.5	3.15	- 5	3.0	2.85	- 8	9.6	- 9.18
-10	13.3	-11.48	-13	3.6	3.33	- 8	1.7	- 1.67	2 10			6	2.5	- 2.71	9	5.1	5.41
-12	2.9	- 2.67	-14	2.3	1.63	9	3.5	3.66	0			7	3.6	- 3.52	- 9	3.4	- 2.78
-14	5.7	5.14	-15	2.4	1.54	- 9	3.2	2.86	1	10.2	-10.28	- 7	5.8	5.50	10	3.2	- 3.44
2 1			2 4			-10	4.0	- 3.46	- 1	4.0	4.38	8	2.6	2.99	-10	4.7	- 4.92
1	10.5	8.66	0	12.4	-12.69	-11	8.0	- 7.41	2	7.3	7.24	- 8	3.8	4.23	-11	4.4	- 4.92
2	4.0	3.42	1	3.3	4.30	12	3.5	3.35	- 2	3.8	3.41	9	3.3	- 2.98	-12	2.9	2.55
3	2.0	3.17	- 1	9.6	9.29	-12	3.0	- 2.91	3	2.4	- 1.86	-11	2.4	- 2.06	-13	4.4	4.32
4	4.0	- 3.85	2	14.5	17.66	-13	2.3	- 1.86	4	2.2	- 1.97	-12	3.6	- 3.52	-14	3.5	3.60
5	2.1	2.70	- 2	27.8	-36.64	-15	2.5	1.83	- 4	6.9	6.91	2 14			-15	2.4	1.59
- 5	14.7	17.10	- 3	5.4	- 5.88	2 7			5	3.3	3.00				3 3		
- 6	14.0	-13.95	4	19.6	22.47				- 5	4.9	- 4.47	1	2.5	2.31			
7	3.2	- 2.82	- 4	3.9	4.57	0	7.5	6.55	6	5.8	- 5.67	2	3.9	3.42	0	14.7	13.54
- 7	1.4	2.25	- 5	2.2	- 1.65	- 1	3.5	- 3.27	- 6	7.1	6.70	- 2	7.1	- 7.10	1	8.4	- 7.18
- 8	1.5	- 1.22	6	1.8	1.14	2	2.7	- 2.65	7	2.1	- 1.60	- 3	4.9	- 5.31	2	6.6	6.19
- 9	8.0	- 8.41	- 6	16.8	20.30	- 2	5.1	- 4.36	- 7	4.9	- 4.13	4	2.2	2.36	3	6.7	6.74
10	8	- 2.62	7	3.1	- 2.60	3	5.3	5.22	8	2.4	- 2.22	5	2.2	- 2.14	- 3	13.0	12.32
-10	2	3.77	- 7	5.2	4.61	- 3	3.8	- 3.90	- 8	2.2	1.79	- 6	3.1	3.32	4	8.6	- 8.92
11	3.8	4.17	8	11.5	-12.09	4	2.2	2.66	-10	7.0	- 6.43	- 7	6.4	6.61	- 4	2.4	2.10
-11	4.2	- 4.22	- 8	5.0	- 4.96	- 4	5.0	- 4.98	-11	3.1	2.66	8	3.1	- 2.97	5	6.9	6.21
-12	2.7	2.02	9	2.2	1.57	- 5	5.9	5.37	-14	2.8	2.89	9	2.8	2.45	- 5	1.5	1.12
-15	4.6	4.26	- 9	1.7	- 1.49	- 6	13.0	13.23	2 11			-11	3.4	- 3.05	6	4.2	- 4.19
			-10	4.9	- 3.89	7	4.9	- 4.62	0			-12	2.5	- 2.15	- 6	3.1	3.51
2 2			-12	4.0	3.95	- 7	7.0	6.73	1	4.1	3.87	2 15			7	2.1	2.30
1	4.5	4.24	2 5			- 8	2.7	3.39	- 1	2.7	2.23				- 7	4.7	- 5.00
2	10.2	11.69				- 9	3.7	- 3.20	2	12.8	-13.64	- 2	3.1	- 2.58	8	2.0	- 1.58
3	5.6	- 5.29	0	6.3	5.08	10	3.2	3.04	3	4.8	4.58	- 6	4.4	3.69	- 8	3.8	- 3.58
4	11.9	12.33	1	6.4	- 5.70	-10	4.6	- 4.16	- 3	8.0	8.00	- 7	4.6	3.96	9	4.7	- 4.99
- 4	4.8	5.86	- 1	19.9	-26.77	11	2.3	1.38	4	5.0	- 4.56	- 8	2.6	2.61	- 9	2.5	- 1.92
						-11	5.5	- 5.15	- 4	5.5	- 5.46	-10	2.8	- .93	-10	2.1	1.41
						12	2.7	- 2.57		3.6	- 3.40	-11	3.2	- 2.54	-13	3.8	3.70

Table 4 (*cont.*)

3 4		3 7		3 11			3 16			4 3			4 7						
0	1.8 - 1.11	- 7	3.6 - 3.92	0	5.8	5.85	2	3.2 - 2.80		0	5.9	5.02	0	6.8 - 7.76					
1	3.0 - 2.93	- 8	4.6 4.61	1	5.5 - 5.33		- 2	2.3 - .04		1	6.9 - 6.48		1	7.9 - 7.63					
- 1	1.7 .78	9	2.8 - 2.40	2	4.3	4.70	- 3	3.5 - 3.42		2	8.6 - 7.83		- 1	6.2 5.41					
2	10.6 -10.98	- 9	9.4 -10.18	- 2	2.9 - 3.57		- 4	4.0 4.52		3	1.7 - 1.65		2	8.6 8.23					
- 2	4.4 - 3.42	-10	4.1 - 4.08	4	3.9 - 3.97		- 5	3.3 3.08		4	2.5 2.42		- 2	7.4 - 6.63					
3	3.4 3.82	-13	3.6 3.68	5	4.7 5.14		- 6	3.6 3.73		- 4	5.5 3.67		3	9.5 -10.20					
- 3	1.8 - .82			6	4.1 - 3.88		- 7	2.4 2.42		5	2.6 2.94		- 3	10.8 10.94					
4	8.5 8.78	3 8		- 8	2.4 - 1.44		- 8	2.5 - 2.99		6	2.8 2.97		5	2.8 3.14					
- 4	2.6 - 2.03	0	17.6 -18.41	9	3.0 - 2.53		- 9	2.5 .39		- 6	3.7 3.01		6	2.9 - 3.07					
- 5	3.7 - 3.89	1	8.6 8.40	- 9	3.1 - 2.79		-10	3.6 - 3.29		- 7	11.8 -12.77		7	6.1 6.45					
6	4.6 4.90	- 1	5.9 - 5.94	-11	2.4 1.74					- 8	11.5 -12.80		- 7	9.2 - 9.38					
- 6	3.6 3.41	2	1.6 - 1.43	-13	2.8 2.06		3 17			- 9	4.4 - 4.39		- 8	7.8 8.18					
7	1.9 - 2.00	- 2	1.6 1.31	-14	2.6 1.76		1	3.6 - 3.74		-10	2.2 - 1.82		-11	4.7 4.31					
- 7	2.4 2.48	- 3	6.3 - 5.55	3 12			2	3.1 3.12		-11	7.6 6.92		-12	2.1 - 2.14					
8	5.5 - 6.32	4	6.0 6.02				- 3	3.4 3.04		-12	4.3 4.02		4 8						
- 8	7.0 - 7.21	- 4	18.3 20.22	1	2.4 - 1.93		4	2.5 1.08		-13	4.8 4.64								
9	2.1 2.27	- 5	8.8 8.00	- 2	2.1 .15		- 4	3.6 - 3.16		-16	3.1 .94		0	4.1 - 3.53					
- 9	2.4 - 1.81	6	3.4 3.36	3	3.6 3.60		5	2.5 1.71		4 4			- 1	1.7 - 1.58					
10	2.2 - 2.06	- 6	5.3 5.89	4	3.0 2.90		- 5	3.7 3.63					2	11.1 -11.94					
-10	3.6 3.24	- 7	2.0 1.98	- 5	3.1 - 2.78		6	3.3 - 3.13		1	1.9 - 1.48		- 2	9.5 9.70					
-12	5.6 5.77	- 8	7.9 - 7.80	6	2.7 2.08		- 6	2.8 2.48		- 1	4.6 - 3.81		3	2.6 2.34					
-13	2.5 1.92	9	2.5 - 1.93	- 6	2.1 - 2.03		- 8	2.5 1.90		2	4.4 - 3.95		- 3	4.2 - 4.18					
3 5		10	2.4 - 1.97	7	2.3 - 2.33		- 9	2.9 - 2.62		- 2	14.2 12.57		4	3.5 - 3.63					
		-10	9.3 - 9.38	- 7	2.1 2.12		-10	2.9 - 2.96		3	2.9 1.79		- 4	6.2 5.87					
0	7.8 - 6.56	-13	2.4 - 2.01	- 8	2.2 - 1.57					- 3	5.1 3.76		5	4.1 4.79					
1	2.8 - 2.08	-14	4.9 4.45	9	3.1 2.36		3 18			4	5.4 5.30		- 5	4.3 4.68					
- 1	10.8 -10.01	-15	2.6 1.82	- 9	3.1 - 2.30		1	3.9 4.18		- 4	5.9 5.37		6	6.8 7.34					
- 2	3.4 - 3.70			-10	2.3 1.75		- 1	2.5 - .91		5	2.7 - 2.53		- 6	5.7 - 5.92					
3	10.5 10.41	3 9		-13	2.5 2.06		- 2	2.5 1.23		- 5	4.0 .97		7	2.0 - 2.07					
- 3	12.8 13.38	0	2.6 2.91	3 13			- 3	2.8 - 2.40		6	1.8 - .46		8	3.7 4.02					
4	3.3 3.04	1	13.9 -13.80				- 4	3.2 2.59		- 6	6.7 - 6.48		- 8	3.7 - 3.48					
- 4	4.9 4.46	- 1	5.7 - 5.34	- 1	3.4 - 2.46		0	3.1 - 1.89		- 8	8.3 - 8.68		- 9	4.1 - 4.28					
5	3.4 3.15	2	5.9 5.93	2	2.1 .80		4 0			-12	8.5 9.05		-10	2.7 2.97					
6	3.1 3.30	- 2	2.1 - 2.69	- 2	4.0 - 3.90					4 5			-14	2.3 - 1.68					
7	2.4 2.40	3	2.5 - 2.34	3	3.0 3.00		2	16.5 -17.77					4 9						
- 7	6.1 - 6.47	- 3	5.1 4.85	- 3	2.8 2.08		4	6.4 - 7.01		1	2.2 - 1.85		0	5.4 - 5.52					
9	4.6 - 4.65	4	1.9 .48	- 4	4.8 4.24		6	10.6 12.56		- 1	2.1 - 1.54		1	10.1 -10.51					
-13	3.2 3.19	5	7.9 8.29	- 8	2.3 - 1.37		- 6	11.7 -10.89		2	6.7 6.14		- 1	6.7 6.35					
3 6		- 5	13.8 14.76	3 14			- 8	8.0 - 7.96		- 2	9.0 - 7.67		- 1	1.7 - .76					
0	11.4 -10.57	6	6.4 - 6.68				-10	7.0 6.85		3	4.6 - 4.38		2	4.2 - 4.63					
1	4.3 - 4.45	- 6	3.4 4.14	0	2.9 - 2.55		-14	2.7 - 2.62		- 3	8.4 7.95		3	9.5 9.91					
- 1	7.2 - 6.81	7	2.1 - .97	1	3.4 - 3.23					- 4	3.8 - 2.82		- 3	2.5 2.54					
2	6.4 - 6.89	- 8	3.1 2.92	- 1	3.2 - 2.81		4 1			- 6	4.4 3.29		4	6.9 6.97					
- 2	3.2 - 2.53	- 9	11.2 -11.36	2	2.2 - 1.86		1	15.6 -17.12		7	3.1 3.34		- 4	3.7 3.67					
4	8.7 8.53	10	2.7 2.76	- 2	2.1 - 1.60		2	8.4 - 7.56		- 7	14.5 -15.94		5	3.4 3.47					
- 4	8.3 8.11	-10	4.6 - 5.09	3	2.5 2.47		3	8.9 - 9.36		- 8	5.7 5.62		7	4.3 - 4.47					
5	5.6 5.55	-13	3.4 3.15	4	3.2 3.44		4	1.7 1.99		-11	7.8 7.85		- 8	4.3 - 2,18					
- 5	8.4 8.54	-14	3.2 2.15	5	2.3 1.98		5	6.1 6.63		-13	2.9 2.89		- 9	2.1 - 1.51					
6	2.9 3.12	-15	2.6 1.53	- 6	3.4 3.18		6	2.5 2.26		-16	3.0 - .46		-12	2.2 1.51					
- 6	7.6 7.78			- 7	2.9 2.72		7	5.5 5.34		4 6			-13	3.7 1.18					
7	2.0 1.58	3 10		- 8	3.0 - 3.07		- 7	5.1 - 6.19					4 10						
8	4.7 - 5.42	0	9.9 - 9.43	3 15			- 8	11.3 -11.13		0	2.2 - 1.48								
- 8	7.8 - 8.47	1	9.6 8.97				- 9	2.3 - 1.82		1	5.3 4.86		0	3.3 - 3.00					
9	3.0 - 3.00	- 2	2.9 2.66	1	2.9 - 2.27		-11	4.1 3.35		- 1	2.7 - 2,36		1	4.0 - 3.75					
-10	3.5 - 3.88	3	2.4 2.20	- 1	5.0 - 4.95		-12	4.0 3.38		2	10.0 - 9.76		- 1	1.9 - 1.73					
-12	5.1 5.36	- 3	5.4 - 5.14	2	2.3 1.61		-13	2.0 1.45		- 2	16.0 16.92		2	4.3 - 4.07					
-13	2.9 - 2.54	4	3.0 2.97	- 2	3.6 - 3.49		-15	3.5 - 3.57		3	5.2 4.60		- 3	8.5 8.44					
3 7		- 4	10.8 11.36	3	3.3 2.88					- 3	14.3 -15.36		4	1.9 - 2.27					
		5	6.2 - 6.48	- 3	4.4 4.45		4 2			4	1.7 1.77		- 4	7.3 7.93					
0	9.9 - 9.60	6	3.8 4.02	4	2.6 1.91		1	8.5 - 7.82		- 4	2.6 2.30		- 5	2.9 3.37					
1	11.6 -11.50	7	3.1 - 3.28	5	2.4 1.19		2	11.3 -10.44		5	3.5 3.78		6	5.0 5.27					
- 1	12.3 -12.15	- 7	1.9 2.24	- 5	5.1 4.69		3	1.8 - 1.38		- 5	2.9 3.46		- 6	3.2 - 3.37					
3	4.4 4.54	- 8	3.7 - 3.50	- 6	3.3 3.27		5	4.6 - 5.09		6	2.5 2.31		- 7	5.4 - 4.75					
- 3	10.1 10.10	- 9	2.7 - 1.98	- 7	2.4 - 1.60		6	5.9 6.72		- 6	7.2 - 6.96		- 8	6.2 - 6.33					
4	7.2 7.76	10	3.5 - 3.20	- 8	2.4 1.58		- 6	9.1 - 8.70		7	3.1 - 2.45		- 9	4.5 - 4.67					
- 4	4.4 - 3.43	-10	3.3 - 3.02	- 9	3.1 - 2.55		- 7	9.6 - 8.80		7	7.1 7.40		-10	2.8 2.69					
5	6.7 6.76	-11	3.1 - 3.03	3 16			- 8	9.3 - 9.40		- 8	4.2 - 4.19		-12	2.8 1.27					
- 5	14.7 17.00	-12	2.4 - .50				-10	3.9 3.94		-12	6.0 5.89		-13	3.9 3.43					
6	1.9 .29	-13	2.5 1.41	0	4.4 - 4.00		-12	5.0 4.54		-13	2.9 - 2.59								
- 6	1.9 2.83	-14	3.6 3.07	1	3.7 3.43		-13	5.1 4.98											
		-15	2.6 2.14	- 1	3.5 - 3.16														

Table 4 (*cont.*)

4 11			5 1			5 4			5 8			5 13			6 3				
1	5.0	- 4.94	0	2.2	1.59	7	1.8	1.30	1	4.0	- 4.23	2	2.7	- 2.84	- 7	4.4	4.45		
- 1	3.0	2.25	1	2.2	- 1.24	- 7	4.2	- 4.43	- 1	2.5	1.81	- 2	2.8	2.39	-10	3.2	- 2.91		
2	3.9	- 3.01	2	4.6	- 4.51	8	4.2	4.92	2	3.0	- 3.00	3	3.9	- 4.09	-13	2.1	- 2.33		
- 2	2.2	1.78	4	2.1	- 1.62	- 8	2.0	2.12	- 2	2.1	- .57	4	3.5	3.77	-14	2.5	1.19		
3	1.9	1.66	5	2.2	- 1.72	-10	7.6	8.15	- 3	1.5	- .80	- 5	3.9	- 4.29	6 4				
- 3	5.2	5.04	- 5	10.5	- 9.42	-12	1.9	1.58	- 4	2.2	- 1.56	- 7	3.3	- 3.79					
- 4	3.5	4.14	- 6	4.9	4.17	-15	2.1	.58	- 5	2.7	- 2.64	-11	3.4	3.71	0	5.6	4.70		
5	2.0	2.10	7	3.3	4.03	-16	2.4	- 2.49	- 6	3.0	2.68	-12	3.5	3.71	2	5.7	5.99		
- 8	6.4	- 7.14	8	1.8	1.10	5 5			- 7	2.9	2.29	5 14			- 2	3.3	- 3.16		
- 9	4.4	- 4.18	- 9	7.3	6.99				- 9	2.0	- 1.68				3	1.8	- 2.53		
-11	2.2	2.02	-10	4.3	- 3.77	0	6.3	- 5.16	-10	2.8	2.72	0	2.2	1.39	4	7.6	- 7.16		
-12	3.7	2.20	-14	2.0	.58	1	3.7	3.52	-13	2.3	1.99	1	2.6	- 1.77	- 4	2.3	- 1.74		
4 12			-15	2.8	- 2.51	- 1	17.2	18.59	-14	3.2	- 3.12	- 1	2.7	- 2.24	6	5.1	- 4.31		
			-16	2.1	1.37	3	11.3	-12.11	-15	2.2	- 1.76	- 2	3.3	3.12	- 6	3.2	- 2.36		
- 1	3.5	- 3.52	5 2			4	4.3	4.09	5 9			- 3	1.9	2.09	- 7	2.2	- 1.82		
3	2.0	1.60				- 4	3.7	3.26				- 4	1.9	- 1.64	- 8	4.4	4.34		
- 3	3.4	3.30	0	10.2	8.33	5	2.3	- 2.50	1	1.8	- 1.37	- 6	4.3	- 4.22	-11	2.0	1.64		
- 4	3.4	3.19	1	5.9	5.65	- 5	9.0	- 8.45	- 1	1.6	- .72	- 7	3.4	- 3.72	-12	3.6	- 4.11		
5	2.7	- 2.39	2	6.1	- 5.55	6	1.8	1.67	- 3	3.0	2.24	-11	3.1	2.83	6 5				
- 6	3.0	- 3.05	3	3.1	- 2.74	- 6	3.2	- 2.73	4	2.0	- 1.89	6 0							
- 8	5.3	- 5.16	4	5.8	- 5.63	7	1.9	1.17	- 4	3.0	2.98				0	4.1	3.55		
-11	2.8	- 1.96	- 4	5.5	- 4.88	- 7	7.8	- 8.20	- 5	4.8	- 5.17	0	9.1	9.31	1	4.5	4.42		
-12	2.6	3.69	5	4.0	- 4.19	8	1.9	- 1.71	- 9	4.0	4.29	2	1.7	- 1.23	- 1	0.2	8.50		
4 13			- 5	4.5	3.94	- 8	2.6	- 2.43	-10	1.9	.25	- 8	10.5	9.24	- 2	2.3	.97		
			6	2.3	1.82	- 9	3.4	3.44	5 10			-10	6.0	5.44	- 3	7.4	- 6.55		
2	2.0	1.54	- 6	9.0	- 8.43	-10	2.4	1.67				-12	3.4	- 2.63	- 4	6.4	- 5.52		
- 2	4.8	- 4.65	7	2.9	3.46	-11	8.2	9.91	0	5.9	5.74	-14	7.0	- 7.54	- 5	4.7	- 4.55		
3	2.3	- 1.64	8	2.4	2.11	-12	3.1	3.49	2	4.1	- 4.22	6 1			- 6	2.7	- 2.46		
- 3	3.1	2.75	-10	7.8	7.43	-13	2.0	- 2.46	- 2	2.8	2.34				- 7	4.5	4.75		
- 4	2.5	- 1.39	-11	5.6	- 5.34	-15	3.3	- 2.91	3	1.8	- 1.58	0	6.6	- 5.90	- 8	2.4	1.84		
- 6	4.5	4.31	-12	1.8	1.15	-16	2.2	- 2.17	- 3	2.7	2.98	1	7.1	6.45	- 9	1.9	- 1.71		
- 7	5.6	- 5.74	-13	2.1	- 2.17	5 6			4	2.7	- 3.07	2	1.9	- 1.74	-10	2.2	2.18		
			-14	4.1	- 4.10				- 4	2.4	- 2.35	3	2.0	- 1.96	6 6				
4 14			-15	3.3	3.02	0	3.7	3.18	- 5	1.9	1.82	5	4.0	- 4.39					
0	2.0	.73	-16	2.1	- .98	1	6.0	- 5.99	- 6	1.9	- 1.82	- 5	9.7	- 8.69	0	4.5	4.30		
- 1	3.5	- 4.22	5 3			- 1	1.4	- 1.41	- 9	2.1	- 1.74	- 6	1.6	.13	1	4.2	3.95		
2	3.5	- 3.49				2	1.7	- 1.26	-10	4.8	5.20	- 7	2.8	2.69	- 1	3.9	3.56		
- 2	6.7	7.07	0	1.3	- .82	- 2	9.2	8.77	-11	2.6	- 2.18	- 9	12.5	13.72	2	2.0	2.31		
3	3.6	3.85	1	1.9	1.59	3	3.0	3.01	5 11			-10	2.8	- 2.48	4	4.3	- 5.12		
- 3	3.4	- 3.12	- 1	21.4	19.03	4	4.2	- 4.15				-13	5.9	- 6.48	- 4	3.8	- 3.35		
- 6	3.1	- 3.09	2	6.3	- 6.58	- 4	4.3	- 4.33	0	2.8	- 2.68	-14	5.1	1.04	- 5	8.2	- 7.53		
- 7	3.1	2.97	- 2	4.0	2.90	5	4.5	4.97	- 1	7.3	7.16	6 2			- 6	3.9	- 3.52		
			3	10.3	-10.57	- 6	10.2	-11.14	2	3.4	- 3.90				- 8	4.7	4.99		
4 15			- 3	4.0	2.73	7	2.5	- 2.29	- 2	2.4	2.51	0	7.6	7.42	- 9	5.4	5.25		
0	2.7	- 2.61	- 4	3.7	- 3.09	- 7	2.5	- 2.75	3	2.5	- 2.65	1	6.6	- 6.16	-10	4.3	4.51		
1	2.1	- .84	5	2.6	- 2.57	8	3.6	3.97	- 3	3.0	3.00	- 1	3.8	- 2.86	-12	3.5	- 4.06		
- 1	2.4	1.58	- 5	13.3	-13.32	- 8	2.2	2.11	- 4	2.3	1.68	2	2.8	2.71	6 7				
2	3.0	2.78	6	2.3	- 1.50	-10	4.0	4.05	- 5	8.7	- 9.31	3	3.2	- 3.32					
- 2	3.9	- 3.89	- 6	4.9	4.75	-11	5.2	5.72	- 7	4.2	- 4.04	4	1.8	- 2.34	0	5.8	5.35		
3	4.9	- 5.03	7	2.5	2.23	-13	2.2	2.25	- 9	4.2	4.37	- 4	12.9	-10.35	1	2.9	2.70		
- 3	3.0	2.87	- 7	8.3	- 8.67	-15	3.3	- 2.78	-10	2.7	- 2.62	5	3.8	4.27	- 1	3.8	3.80		
- 7	5.0	- 4.64	- 9	5.9	5.77	-16	2.2	- 1.91	-11	2.0	2.46	- 5	10.4	8.56	- 2	1.9	- 1.99		
4 16			-10	4.8	- 4.94	5 7			-12	2.1	1.32	6	2.3	- 2.29	- 3	4.3	- 4.15		
			-11	7.6	8.65				5 12			- 6	1.8	- .43	- 4	4.9	- 4.65		
2	3.7	- 4.31	-12	1.8	.73	0	2.4	- 1.72				- 7	3.6	- 3.20	- 5	7.5	- 7.63		
- 2	4.9	4.79	-13	2.6	- 2.60	- 1	2.5	2.11	0	6.1	6.50	- 8	8.0	7.17	- 6	1.8	- 2.39		
- 5	2.2	2.46	-14	2.0	.66	2	4.1	4.08	- 1	2.9	- 2.93	- 9	6.1	- 6.13	- 7	3.1	3.33		
4 17			-15	3.4	- 3.08	- 2	2.1	- 1.64	2	2.6	- 1.92	-11	2.2	2.43	- 8	2.1	- 2.31		
			-16	2.2	.88	3	3.7	- 3.62	- 2	5.8	6.16	-12	3.4	- 3.17	- 9	6.9	6.99		
0	2.9	- 3.33	5 4			4	1.9	1.71	- 3	4.2	4.86	-14	2.5	- 2.92	-10	3.8	4.51		
1	2.3	- 2.19				- 4	5.9	5.44	4	4.6	- 4.68	6 3			-13	3.2	- 3.81		
- 1	2.2	.54	0	9.7	8.91	- 5	1.9	- 1.77	- 4	3.1	- 3.26				6 8				
- 3	2.2	2.28	- 1	3.3	- 2.76	- 6	4.9	- 4.62	- 5	4.3	4.33	0	7.5	- 6.75					
- 4	3.2	3.06	2	2.8	- 2.60	- 8	2.5	- 2.58	- 6	7.1	- 7.80	1	6.9	6.84	0	4.3	4.87		
			- 2	16.6	17.24	- 9	2.7	2.70	- 7	4.3	- 4.80	- 1	6.4	5.70	1	2.1	- 2.16		
5 0			- 3	4.2	4.01	-10	4.9	4.52	-10	3.9	4.38	2	1.9	- 1.99	- 3	5.2	5.12		
0	7.4	5.71	4	8.6	- 8.57	-11	1.9	1.86	5 13			- 2	6.6	5.84	- 4	8.5	- 8.94		
2	6.5	- 6.96	- 4	7.0	- 6.77	-13	2.0	- 1.31				- 3	9.6	- 7.65	- 5	3.2	- 3.54		
4	2.0	- 1.92	5	1.9	.96	-15	2.7	- 2.24	0	4.9	- 4.70	- 4	8.6	7.07	- 8	6.1	6.35		
- 6	8.5	6.71	- 5	4.5	3.86	-16	2.5	- 1 72	- 1	6.9	6.90	- 5	3.4	- 3.93	-10	4.7	4.97		
-10	5.8	5.19	6	1.8	.10							- 5	3.9	- 3.72	-12	2.4	- 2.59		
-14	5.9	- 5.83	- 6	19.9	-23.39										-14	4.5	- 4.96		

Table 4 (*cont.*)

6-9			7 0			7 3			7 6			7 9			7 12		
0	1.9	1.76	0	2.6	2.29	0	1.4	1.14	0	2.3	2.34	0	2.2	2.43	-7	1.9	1.66
1	4.3	4.53	2	6.8	7.31	1	1.4	.85	1	1.6	1.56	1	4.1	4.78	-11	1.8	.79
2	3.2	3.44	4	2.6	2.86	-1	1.3	.79	2	3.2	3.40	-1	3.0	3.10	-12	1.8	1.54
-3	4.4	4.16	-6	8.4	6.43	2	2.6	2.22	-2	6.4	6.24	2	1.8	1.65			
-4	4.8	4.74	-8	9.7	9.57	-2	2.8	2.16	-3	3.9	3.77		2.9	2.96	7 13		
5	2.1	2.75	-10	4.4	4.40	-3	2.2	1.86	-5	2.5	2.24	-3	6.4	6.36	-6	2.5	2.40
-5	4.4	4.52	-12	3.2	3.63	4	1.7	1.40	-6	5.8	5.80	4	1.9	1.83	-7	1.7	1.74
6	2.2	2.43	-14	2.5	2.36	-6	2.4	2.31	-7	6.3	5.97	-4	2.7	2.95	-11	2.4	2.21
-7	2.2	2.07	7 1			-7	4.0	3.42	-10	2.1	1.75	-5	2.5	2.70	7 14		
-8	3.8	4.22				-8	4.5	4.43	-12	3.3	3.64	-7	4.0	4.07			
-9	7.6	8.82	0	1.7	.63	-11	4.0	4.13	-13	2.2	1.97	-8	2.9	3.26	-1	1.9	1.79
-13	3.4	4.27	1	7.2	7.54	-12	4.7	5.08	-16	2.9	2.83	-12	1.7	1.54	-2	2.5	2.73
6 10			-1	6.0	4.80	-15	2.2	2.12	7 7			-13	2.0	2.22	-5	1.7	1.45
			2	1.6	1.54	-17	2.0	1.71				-14	2.0	1.55	-6	2.9	2.89
0	4.1	4.38	3	4.1	4.31				0	2.8	2.79	7 10			-7	1.9	1.37
1	4.9	5.41	4	1.5	1.36	7 4			1	3.1	2.83				-11	1.8	1.22
-3	4.7	4.92	-5	4.3	4.22				-1	4.4	4.30	0	1.8	1.64	-12	2.0	1.81
-4	7.1	7.83	-7	8.4	7.58	0	3.5	3.00	2	2.5	2.71	-1	2.0	1.71	7 15		
-5	3.1	2.65	-8	4.5	4.27	1	1.9	.83	-2	3.8	3.52	2	2.5	2.21			
-6	2.0	1.92	-9	1.4	.91	-1	2.2	1.64	3	4.1	4.31	-2	1.7	1.55	-1	2.6	2.22
-7	2.2	2.55	-11	3.3	3.32	-3	1.8	1.09	-3	6.6	6.47	3	1.8	1.68	-2	2.0	1.76
-8	3.8	4.37	-12	4.4	4.32	4	1.6	1.45	-4	2.3	2.36	-3	2.3	2.02	-3	1.9	1.91
6 11			-13	2.8	2.84	-4	1.5	1.34	-7	7.0	7.62	-4	3.1	3.29	-4	1.7	1.11
			-15	2.2	2.20	-6	3.4	3.28	-8	2.5	2.35	-5	1.5	1.35	-6	2.0	1.79
0	3.2	3.50	-16	1.8	.52	-7	2.3	1.73	-11	4.1	4.39	-7	3.3	2.92	-7	3.0	3.41
1	4.5	4.95				-9	1.9	.41	-12	3.4	2.53	-8	4.0	4.26	-11	2.5	2.28
2	2.9	2.81	7 2			-12	3.3	3.46	-15	1.8	1.73	-9	2.7	2.55	7 16		
-2	3.7	4.11				-16	3.2	3.42	7 8			-13	2.7	3.02			
-3	3.1	3.41	1	2.2	1.93	7 5						7 11			-1	2.0	1.59
-4	3.4	3.80	-1	4.0	3.42				1	2.1	1.69				-2	2.9	3.37
6 12			2	4.2	3.87	1	1.4	1.32	2	4.8	5.33	1	2.3	2.08	-5	1.8	2.10
			-2	6.4	4.88	-2	2.1	1.62	-2	7.3	7.61	-2	1.6	.76	-6	2.0	2.34
0	2.8	2.92	3	2.1	2.36	3	1.5	1.17	3	1.8	.95	-3	1.6	1.43			
2	2.4	2.38	-6	5.1	4.34	-5	1.9	1.53	-3	1.5	1.34	-8	2.8	2.90			
-2	2.0	.82	-7	8.3	7.85	-6	2.0	1.43	4	2.1	1.94	-11	1.7	.79			
3	2.2	2.94	-8	5.4	5.18	-7	4.9	4.77	-4	4.2	4.15	-12	3.2	2.88			
-4	2.5	2.46	-10	3.2	3.04	-8	3.0	2.80	-5	2.9	3.06	-13	2.0	2.07			
6 13			-12	3.2	3.40	-11	4.9	5.33	-6	4.9	5.09						
			-13	3.4	3.33	-12	2.1	2.23	-7	2.5	2.64						
-1	3.4	2.71	-14	1.7	9.6	-15	2.0	2.03	-8	4.7	5.17						
-1	3.0	2.97	-16	2.0	1.89	-16	1.8	.19	-9	2.6	3.01						
-4	3.4	2.06	-17	2.0	2.37	-17	1.8	1.48	-10	2.4	2.37						
									-12	2.8	2.63						
									-13	1.7	1.18						

as to chlorine positions, and thence through Fourier syntheses to a rough structure. Oxygen positions appeared on the earliest electron-density projections, and it seems unnecessary to record the course of the determination in more detail here.

Patterson and Fourier syntheses were computed by means of the TDF40–80 Program for the IBM-650 written by D. R. F. (unpublished, but a later version, TDF2, is available upon request). Refinement procedures, first two-dimensional and later three-dimensional, were made by means of 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 (ORXLS) of Busing & Levy (1959*a*), with anisotropic temperature factors, was used on the MURA IBM-704 at Madison, Wisconsin. In the final refinement variable weighting factors were used proportional to F_o^2 for $I_o < 16I_{\min}$ and inversely proportional for $I_o > 16I_{\min}$. Final parameters (Tables 1, 2 and 3) 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 4.

Throughout this work, the scattering factors used were those of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955). Corrections for anomalous dispersion were made, following Dauben & Templeton (1955).

Discussion of the structure

General description

$LiCuCl_3.2H_2O$ is made up of nearly planar ions $[Cu_2Cl_6]^{2-}$ of approximately D_{2h} symmetry. The Cu–Cl distances within the ion are ~ 2·3 Å, and the ions are connected into $(Cu_2Cl_6^{2-})_x$ chains through two Cu···Cl

links of about 2·9 Å, 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(2) is approximately square planar, but in addition each copper atom has a chlorine atom above the plane at 2·9 Å, and a water molecule (O1) below at 2·6 Å, so that the overall configuration about Cu(2) is approximately a tetragonally deformed octahedron, a predominant feature of Cu(2) crystal chemistry.

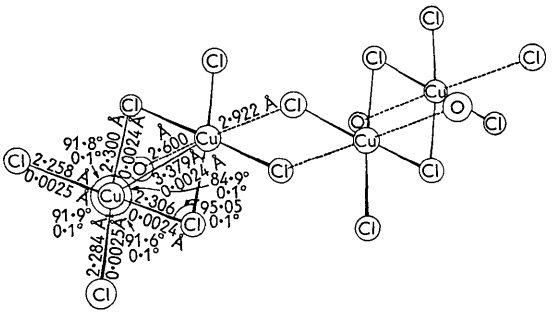

Fig. 1. The $[Cu_2Cl_6]^{2-}$ ion in perspective drawing.

Half the water molecules are bound to Cu(2) and half appear between chains, grouped in pairs, which suggest that they form part of a polyhedron about the lithium ion. We did not obtain a full three-dimensional Fourier synthesis for the structure, and hence we have not seriously attempted to find Li and H positions since a neutron diffraction investigation by Dr S. C. Abrahams, under way at Brookhaven National Laboratory, should provide unambiguous positions.

Table 5. *Interatomic distances* ≤ 3·5 Å

Bond	Distance	σ
Cu–Cl(1)	2·259 Å	0·0025 Å
	2·922	
Cu–Cl(2)	2·285	0·0025
Cu–Cl(3)	2·301	0·0024
	2·307	0·0024
Cu–O(1)	2·600	0·0084
Cu–Cu	3·399	0·0029
O(1)–Cl(1)	3·261	0·0077
O(1)–Cl(2)	3·408	0·0084
O(1)–Cl(2)	3·396	0·0073
O(1)–Cl(2)	3·201	0·0083
O(1)–Cl(3)	3·375	0·0080
O(1)–Cl(3)	3·407	0·0082
O(1)–Cl(3)	3·539	0·0081
O(1)–O(2)	3·058	0·0105
O(1)–O(2)	3·066	0·0108
O(2)–Cl(1)	3·195	0·0075
O(2)–Cl(2)	3·365	0·0074
(O2)–Cl(2)	3·201	0·0069
O(2)–Cl(2)	3·365	0·0074
O(2)–Cl(3)	3·340	0·0077
O(2)–O(2)	2·876	
Cl(2)–Cl(1)	3·266	0·0035
Cl(2)–Cl(3)	3·294	0·0036
Cl(3)–Cl(1)	3·275	0·0037
Cl(3)–Cl(3)	3·112	0·0044

Table 6. *Bond distances averaged over thermal motion*

Bond *A*–*B*	Atom *B* riding on atom *A*	Atom *A* riding on atom *B*	Independent motion	σ
Cu–Cl(1)	2·258 Å	2·260 Å	2·281 Å	0·0025 Å
Cu–Cl(2)	2·284	2·286	2·307	0·0025
Cu–Cl(3)	2·300	2·302	2·323	0·0024
Cu–Cl(3)	2·306	2·308	2·329	0·0024
Cu–O(1)	2·597	2·604	2·617	0·0084

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^{2+} and Li^+ ions so that no very long range cubic or hexagonal arrangement of the layers is maintained. A complete list of interatomic distances, as calculated by the ORXFE program of Busing & Levy (1959*b*), is given in Table 5; a comparison of bond distances, averaged over thermal motion, is given in Table 6. 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 $[Cu_2Cl_6]^{2-}$ *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 Cl(1)–Cu–Cu, Cl(2)–Cu–Cu and Cl(3)–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(1) forms an external Cu–Cl bond of 2·258 Å within the $[Cu_2Cl_6]^{2-}$ ion and a weaker bond of 2·922 Å to the copper of a neighboring $[Cu_2Cl_6]^{2-}$. Cl(2) forms an exterior Cu–Cl bond of 2·284 Å with no further bond to copper. Standard deviations of 0·0025 Å indicate that the difference between these two Cu–Cl bonds is real, and since it is in the opposite direction to that expected, we suppose that Cl(2) is more strongly hydrogen bonded than Cl(1). There are two crystallographic Cu–Cl(3) bridge bonds of 2·300 and 2·306 Å. The difference is of doubtful significance. Bond angles are given in Fig. 1. They deviate significantly from the right angles expected for most descriptions of the bonding to Cu(2), 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 $CuCl_2.2H_2O$ (Peterson & Levy, 1957) for non-bridged Cu–Cl bonds (2·275 Å) and bridges in $CuCl_2$ (Wells, 1947*a*) (2·3 Å).

Color and structure

As noted above, $LiCuCl_3.2H_2O$ 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 $Cu\diagup Cl\diagdown Cu$ bridges where the bridge angle is $\sim 90°$ and where both bridge bonds are $\sim 2{\cdot}3$ Å. These include $CuCl_2$ (anhydrous) (Wells, 1947*a*), $CsCuCl_3$ (Wells, 1947*b*), $KCuCl_3$ (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(2) are chlorine. If in all of the $Cu\diagup Cl\diagdown Cu$ bridges, there is one long bond $\sim 2{\cdot}9$ Å, then the color is blue. A further study of the colors of Cu(2) compounds is under way, but data on the pleochroism in $LiCuCl_3.2H_2O$ are as follows.

Crystals of $LiCuCl_3.2H_2O$ grow as elongated prisms. The principal edges are parallel to *a*, the most prominent faces are {011}, with faces {010} and {001} also observable on most crystals. Faces terminating the prisms were not well developed, and the hygroscopic nature of the crystals made it possible to identify only the most prominent face, which is {112}.

In some crystals it was possible to observe the crystals with polarized light normal to (010). When so viewed the crystals are dark garnet-red with the electric vector 30° to *a* and approximately parallel to [102], while they are lighter, amber-colored with the electric vector normal to this direction. When the crystals are viewed through the face (011) the result is similar, but in a thin crystal when the projection of the electric vector is normal to [102] the color is a green-yellow.

For maximum absorption the electric vector is, within the accuracy of our observation, parallel to the Cu–Cu vector between copper atoms in the dimer. It is noteworthy that in $CuCl_2$ (anhydrous) maximum light absorption occurs when the electric vector is parallel to the chains.

* *Note added in proof.* For complete structures of $KCuCl_3$ and NH_4CuCl_3 see Willett, Dwiggins, Kruh & Rundle (1963).

Magnetic properties

$LiCuCl_3.2H_2O$ remains paramagnetic to about 5·9 °K, where magnetic ordering, presumably antiferromagnetic, takes place (Vossos, Jennings & Rundle, 1960). As noted above, Dr S. C. Abrahams has kindly consented to study the nature of the magnetic ordering by neutron diffraction.

Our indebtedness to Drs Busing and Levy for IBM 704 programs will be clearly evident from the many references to them throughout the text.

References

Berghuis, J., Haanappel, IJ. M., Potters, M., Loopstra, B.O., MacGillavry, C.H. & Veenendaal, A.L. (1955). *Acta Cryst.* **8**, 478.

Buerger, M. (1942). *X-Ray Crystallography.* Chapter 21. New York: Wiley.

Busing, W. R. & Levy, H. A. (1959*a*). *U. S. Atomic Energy Commission Report*, ORNL 59-4-37, Oak Ridge National Laboratory, Oak Ridge, Tenn.

Busing, W. R. & Levy, H. A. (1959*b*). *U. S. Atomic Energy Commission Report*, ORNL 59-12-3, Oak Ridge National Laboratory, Oak Ridge, Tenn.

Chassevant, M. A. (1891). *C. R. Acad. Sci. Paris*, **113**, 646.

Dauben, C. H. & Templeton, D. H. (1955). *Acta Cryst.* **8**, 841.

Donnan, F. G. (1905). *Z. Phys. Chem.* **53**, 317.

Dwiggins, C. W. (1958). *Determination of the Crystal Structure of Potassium Trichlorocuprate*, II. Thesis, University of Arkansas.

Getman, F. H. (1922). *J. Phys. Chem.* **26**, 377.

Meyerhoffer, W. (1892). *Mh. Chem.* **13**, 716.

Peterson, S. W. & Levy, H. A. (1957). *J. Chem. Phys.* **26**, 220.

Vossos, P. H., Jennings, L. D. & Rundle, R. E. (1960). *J. Chem. Phys.* **32**, 1590.

Wells, A. F. (1947*a*). *J. Chem. Soc.* p. 1670.

Wells, A. F. (1947*b*). *J. Chem. Soc.* p. 1662.

Werner, A. (1911). *New Ideas on Inorganic Chemistry.* London: Longmans.

Willett, R., Dwiggins, C. W., Kruh, R. & Rundle, R. E. (1963). *J. Chem. Phys.* **38**, 2429.