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Mn-bearing pinkish epidote from Nakatatsu Mine, Fukui Prefecture

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Abstract Pinkish epidote was found from Nakatatsu Mine, Fukui Prefecture, Japan, and its mineralogical data and crystal structure are described.

The average chemical composition is

$Ca_{1.85}\ Sr_{0.04}\ Al_{2.50}\ Fe_{0.32}\ Mn_{0.04}\ Si_{3.00}\ O_{12}\ (OH)$,

and cell dimensions are $a=8.879(2)$, $b=5.6083(3)$, $c=10.1483(10)$ Å, and $\beta=115.42(4)°$. Least-squares refinement of the structure using X-ray intensity data from a single crystal converged to an R-value of 6.42%, and shows that Fe and Mn are located over $M(3)$ sites and most Sr atoms replace Ca atoms at $A(2)$ sites. Atomic distances are 1.906, 1.883 and 1.812 Å for $M(1)$-O, $M(2)$-O and $M(3)$-O, respectively, and 2.531 and 2.585 Å for $A(1)$-O and $A(2)$-O, respectively.

Introduction

Al-Fe^{3+} and Sr^{2+}-bearing epidotes are known in several metamorphic rocks, such as metagreywacke-quartzofeldspathic schist (Grapes and Watanabe, 1984). These epidotes have been described mainly for petrological aspects. The crystal structures of epidote minerals have been studied by many authors: e. g. Ito(1950), Dollase(1968, 1969 and 1971) and Gabe et al. (1973). However, Mn and Sr locations have not been well established.

Pinkish epidote, which contains Fe, Mn and small amount of Sr, was found from Nakatatsu Mine, Fukui Prefecture, Japan. Chemical composition, mineralogical data and crystal structure of this material are reported.

Experimental

Specimen

The sample was found in debris from Hitokata deposit of Nakatatsu Mine. Optical

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microscopic observation shows that the rock consists of 60% epidote, 20% quartz, 10% calcite and 10% opaque minerals; quartz appears idiomorphic or hypautomorphic, and calcite allotriomorphic. On the surface of the rock, lawmontite is also observed. Most of the pinkish epidote crystals are columnar or acicular elongating along b, and attain up to several mm in length. The optical microscopic photographs of the thin section are shown in plate 1. Optical axial angles measured are $2V(+)=85-95°$.

Chemical composition

Chemical analyses were carried out using an electron microprobe analyzer, model HITACHI XMA-5A. In these analyses, small amount of Sr was detected. Chemical compositions and numbers of cations were calculated based on 12 oxygen atoms per formula unit, assuming perfect stoichiometry for the relative cation proportions (Table 1). The chemical formula averaged over five points in one grain is

$Ca_{1.85}\ Sr_{0.04}\ Al_{2.50}\ Fe_{0.32}\ Mn_{0.04}\ Si_{3.00}\ O_{12}\ (OH)$.

Table 1 Chemical Compositions

	(1)	(2)	(3)	(4)	(5)
SiO_2	39.46	40.38	40.29	39.63	40.18
Al_2O_3	29.31	28.27	26.48	27.85	29.54
$Fe_2O_3^*$	5.78	5.83	5.46	5.69	5.13
MnO	0.70	0.76	0.75	0.58	0.53
CaO	22.33	23.02	23.32	23.13	23.05
SrO	1.25	1.15	1.11	1.12	0.98
Total	98.83	99.41	97.41	98.00	99.41
Numbers of ions on the basis of 12(O)					
Si	2.95	3.01	3.06	3.00	2.97
Al	2.59	2.48	2.37	2.49	2.58
Fe	0.33	0.33	0.31	0.33	0.29
Mn	0.04	0.05	0.05	0.04	0.03
Ca	1.79	1.84	1.90	1.88	1.83
Sr	0.05	0.05	0.04	0.04	0.04

* Fe total as Fe_2O_3.

X-ray studies

Weissenberg and precession photographs indicate that Laue group is $2/m$ and reflections $0k0$ are systematically absent if k is odd. Possible space group is thus $P2_1/m$ or $P2_1$.

A specimen, $0.07\times0.06\times0.05mm^3$ in size, was selected for intensity measurements on a Philips PW 1100 single crystal diffractometer. Cell constants were determined using 25 reflections. Crystal data and information for the structure analysis are given in Table 2. Intensities of 2247 reflections in the range of 2θ from 6 to 70° were measured with graphite monochromatized Mo Kα radiation ($\lambda=0.71069$ Å) and the $\theta/2\theta$ scan mode. Structure factors of 1444 reflections, magnitude of which exceeds corresponding $3\sigma(F_0)$, were used in the following calulations.

Refinement was carried out using the least-squares program *ORXFLS4* (Busing et al. 1962 and Johnson, 1969). Scattering factors for neutral atoms (*International Tables for X-ray Crystallography*, vol. IV, 1974) were used throughout this study. The space group $P2_1/m$ was assumed and initial positional parameters were taken from those by Dollase (1971). R-values with isotropic temperature factors is 6.72%. The occupancy of the M sites and the A sites were also refined (Fig. 1). First of all, the multiplicity of the M sites was refined without chemical constraints, using only the Al atomic form factor. This result (Table 4) suggests that the $M(1)$ and $M(2)$ sites are occupied only by Al, but the $M(3)$ by Al and partly heavier cations, Fe and Mn in this case. In the following calculations, the

Table 2 Crystal Data and information for Structure Analysis

a(Å)	8.879(2)
b(Å)	5.6083(3)
c(Å)	10.1483(10)
β(°)	115.42(4)
V_{calc}	456.42(2)
Crystal System	monoclinic
Space Group	$P2_1/m$
Z	2
D_{calc}	3.63
Radiation Used	MoKα (0.71069 Å), 40kV, 20mA
Monochrometer	graphite
Crystal Size (mm³)	0.07×0.06×0.05
μ (cm^{-1})	26.97
Diffractometer	Philips PW-1100
Scan Type	θ -2θ
2θ Range (°)	6-70
No. of independent reflections measured	2247
No. of independent reflections used for refinement with $F_o > 3\sigma(F_o)$	14444
Final R	6.42%
Final R_w	5.40%

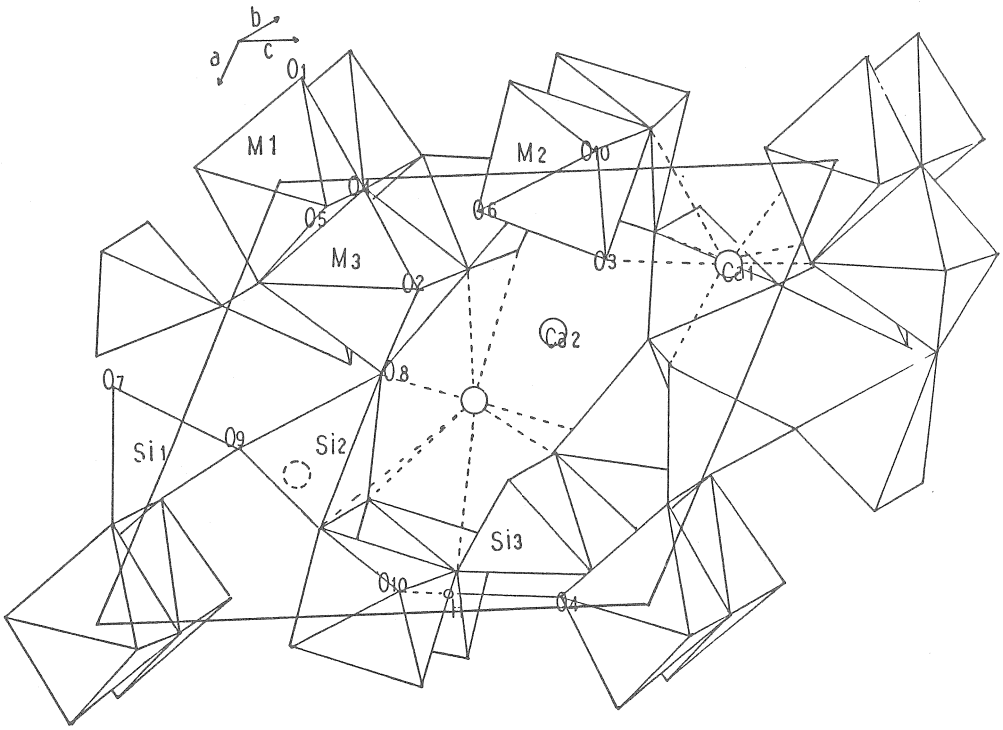

Fig. 1 Polyhedral linkage of epidote
——: Boundary of the Unit Cell

scattering factors for the M sites are assumed as shown in the last column of (a) in Table 4. Then the site occupancy of the A-sites refined with a chemical constraint, Sr=0.04

Table 3 (a) Positional Parameters

	y/a	y/b	z/c
A 1	0.7592(2)	0.75	0.1536(2)
A 2	0.6061(2)	0.75	0.4239(2)
Si 1	0.3389(3)	0.75	0.0478(3)
Si 2	0.6815(3)	0.25	0.2753(3)
Si 3	0.1829(3)	0.75	0.3169(3)
M 1	0.0	0.0	0.0
M 2	0.0	0.0	0.5
M 3	0.2914(2)	0.75	0.2242(2)
O 1	0.2332(4)	0.9965(7)	0.0426(4)
O 2	0.3016(4)	0.9840(8)	0.3526((4)
O 3	0.7911(4)	0.0134(7)	0.3430(4)
O 4	0.0536(6)	0.25	0.1303(5)
O 5	0.0410(6)	0.75	0.1447(5)
O 6	0.0643(6)	0.75	0.4039(6)
O 7	0.5145((6)	0.75	0.1789(6)
O 8	0.5173(7)	0.25	0.3029(6)
O 9	0.6335(7)	0.25	0.1012(6)
O 10	0.0784(6)	0.25	0.4257(5)

The numbers in parentheses represent estimated standard deviations.

Table 3 (b) Anisotropic thermal Parameters $\times 10^{-2}$)

	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Ca 1	0.34(3)	0.58(5)	0.17(2)	0.0	0.17(2)	0.0
Ca 2	0.34(3)	1.05(6)	0.17(2)	0.0	0.11(2)	0.0
Si 1	0.15(3)	0.28(6)	0.09(2)	0.0	0.03(2)	0.0
Si 2	0.19(3)	0.41(6)	0.09(2)	0.0	0.06(2)	0.0
Si 3	0.13(3)	0.35(6)	0.11(2)	0.0	0.04(2)	0.0
M 1	0.16(3)	0.29(6)	0.11(2)	0.01(4)	0.04(2)	0.04(3)
M 2	0.20(3)	0.23(6)	0.13(2)	0.01(4)	0.06(2)	0.0001(9)
M 3	0.15(3)	0.39(5)	0.09(2)	0.0	0.01(2)	0.0
O 1	0.27(5)	0.19(9)	0.28(4)	0.04(6)	0.13(4)	−0.03(5)
O 2	0.23(4)	0.52(10)	0.17(4)	0.12(6)	0.08(3)	−0.04(5)
O 3	0.23(4)	0.37(10)	0.24(4)	0.03(6)	0.02(3)	−0.04(5)
O 4	0.15(6)	0.26(14)	0.18(5)	0.0	0.10(5)	0.0
O 5	0.16(6)	0.31(13)	0.05(5)	0.0	0.01(4)	0.0
O 6	0.29(7)	0.17(14)	0.22(5)	0.0	0.12(5)	0.0
O 7	0.11(6)	0.73(16)	0.21(5)	0.0	0.03(5)	0.0
O 8	0.45(8)	0.83(17)	0.39(6)	0.0	0.30(6)	0.0
O 9	0.64(9)	1.57(21)	0.16(5)	0.0	0.19(6)	0.0
O 10	0.27(7)	0.23(14)	0.16(5)	0.0	0.15(5)	0.0

The numbers in parentheses represent estimated standard deviations.

Anisotropic temperature factors: $\exp\left[-\sum_{i=1}^{3}\sum_{j=1}^{3} h_i h_j B_{ij}\right]$

atoms per formula unit. The final R-value is 6.42% and the parameter shifts are less than one quarter of the corresponding standard deviations. The positional and thermal parameters are listed in Table 3a and b. The structure factors are given in Appendix.

Discussion

Table 4 shows the refined site occupancies for the M and A sites. Sr is mostly distributed over the $A(2)$ sites. The chemical formula is thus calculated as
$(Ca_{0.998}\ Sr_{0.002})\ (Ca_{0.962}\ Sr_{0.038})\ Al_{1.00}\ Al_{1.00}\ (Al_{0.603}\ Fe_{0.376}\ Mn_{0.021})\ Si_3O_{13}H$
based on 12 O and 1 OH.

Tables 5 and 6 show the comparison of A-O and M-O distances with those of other epidote minerals. The chemical formula of other epidote minerals are listed in the bottom of Table 5. Mean M-O distances and their ratio to clinozoisite are also shown in Table 6. The volume of the $A(2)$ sites of the present specimen and piemontite (Dollase, 1969) is larger than that of other epidotes where the $A(2)$ sites are occupied only by Ca. Thus the $A(2)$ site is considered to be enlarged by including large cations as Sr. Clinozoiste (Dollase, 1968) has chemical composition close to Al end-member of Al-Fe-Mn epidotes. The substitution of Fe and Mn might occur more easily in the $M(3)$ site, and therfore, the $M(3)$ -O distances become larger in proportion to the amount of Fe and/or Mn contents.

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Table 4 Site Occupancy

		Multiplicity	Capable Site Occupancy
(a) calculated site occupancies without any constrain			
A(1)		0.501(5)	
A(2)		0.496(5)	
M(1)		0.489(6)**	$Al_{1.000}$
M(2)		0.492(6)**	$Al_{1.000}$
M(3)		0.719(7)**	$Al_{0.603}Fe_{0.376}Mn_{0.021}$
(b) calculated site occupancy in the A sites with chemical constraint as Sr=0.04 atoms per formula*			
A(1)	Ca	0.499(4)	$Ca_{0.998}Sr_{0.002}$
	Sr	0.0009	
A(2)	Ca	0.481(7)	$Ca_{0.962}Sr_{0.038}$
	Sr	0.0191	

* This value is obtained by the chemical analysis shown in Table 1.

**The multiplicities of M sites were calculated using only the Al atomic form factor.

Table 5 Comparison of A-O Distances

Bond	clinozoisite Dollase, 1968	piemontite Dollase, 1969	epidote Gabe et al, 1973	This Study
A(1)				
−O(1)	2.490 Å	2.45(7) Å	2.4780(9) Å	2.471(5) Å
−O(3)	2.369	2.32(5)	2.3449(8)	2.342(5)
−O(5)	2.522	2.55(8)	2.5343(13)	2.543(6)
−O(6)	2.745	2.87(4)	2.7893(10)	2.807(5)
−O(7)	2.284	2.28(9)	2.2841(13)	2.294(6)
−O(9)		3.05	2.9746(6)	2.980(2)
Average*	2.467	2.48	2.4861	2.491
Average**		2.54	2.5781	2.531
A(2)				
−O(2)	2.819	2.71(1)	2.8097(9)	2.806(4)
−O(2′)	2.543	2.54(9)	2.5359(8)	2.806(4)
−O(3)	2.531	2.74(6)	2.5754(9)	2.591(5)
−O(7)	2.267	2.27(8)	2.2616(12)	2.260(6)
−O(10)	2.575	2.54(2)	2.5509(11)	2.551(5)
−O(8)	3.045		3.0294(6)	3.390(8)
Average*	2.579	2.60	2.5465	2.585
Average**	2.625		2.6713	2.734

clinozoisite (Dollase, 1968) ; $Ca_2Al_{2.97}Fe_{0.03}Si_3O_{13}H$

piemontite (Dollase, 1969) ; $Ca_{1.00}Ca_{0.87}Sr_{0.13}Al_{0.80}M_{0.20}-Al_{1.00}Al_{0.17}M_{0.83}Si_3O_{13}H$ for $M=Fe_{0.8}Mn_{0.2}$

epidote (Gabe et al, 1973) ; $Ca_2Al_{2.60}Fe_{0.40}Si_3O_{13}H$

* average of five distances

**average of six distances

Plate 1. Microscopic photographs of epidote, Nakatatsu Mine.

(a) Open nicol

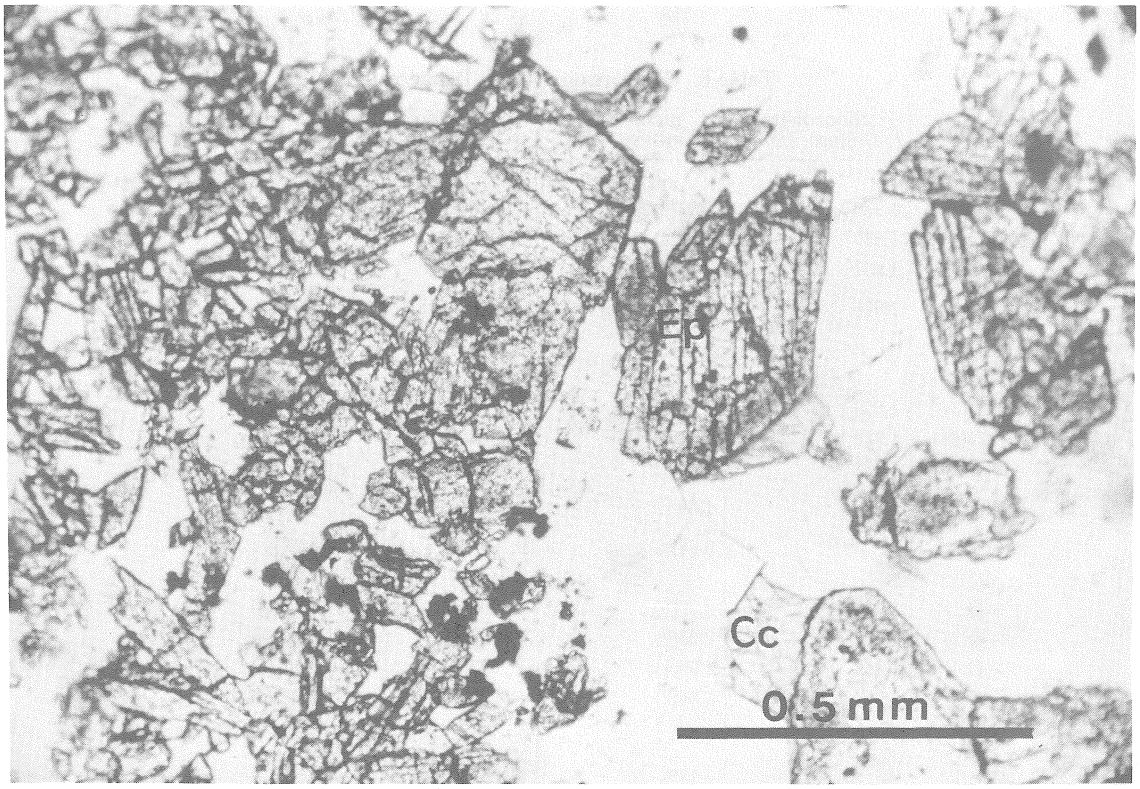
(b) Crossed nicol

E_p : epidote

Q_z : quUrtz

C_c : calcite

(a)



(b)

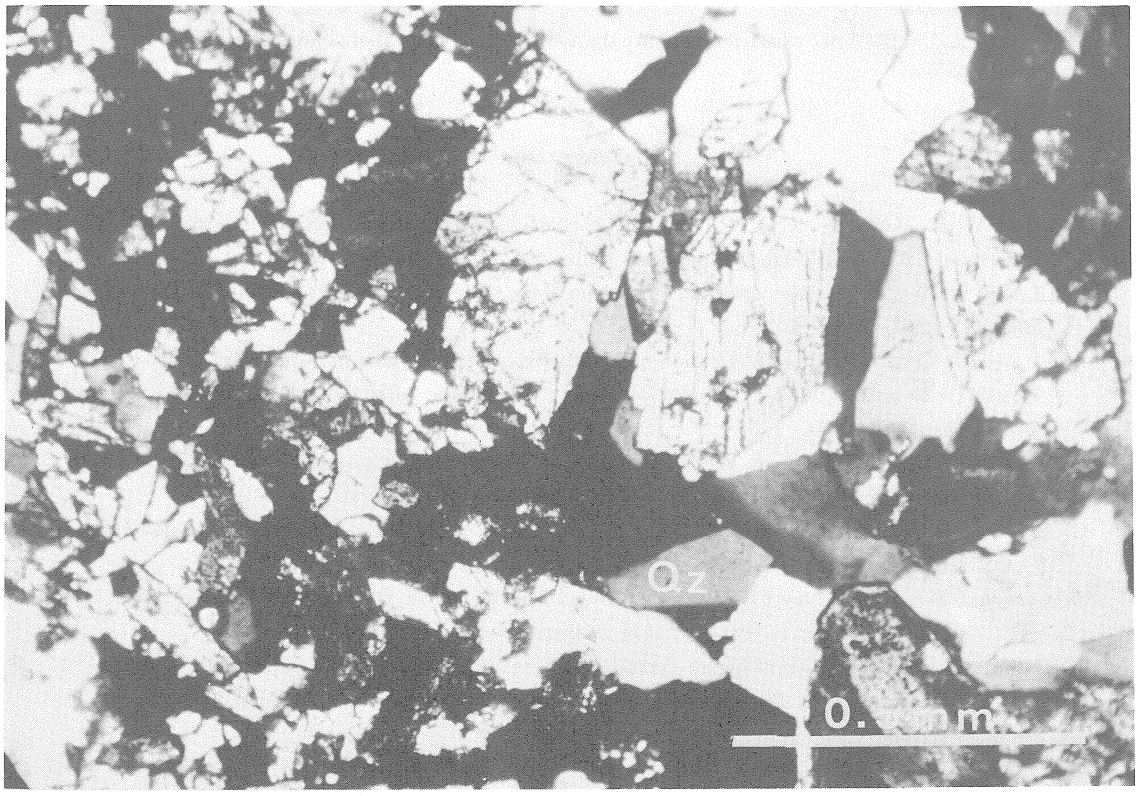


Table 6 Comparison of M-O Distances

Bond	clinozoisite Dollase, 1968	piemontite Dollase, 1969	epidote Gabe et al, 1973	This Study
M(1)				
−O(1)	1.930 Å	1.94(2) Å	1.9316(8) Å	1.925(4) Å
−O(4)	1.850	1.87(3)	1.8466(7)	1.844(4)
−O(5)	1.937	1.98(6)	1.9433(8)	1.948(4)
Average	1.906	1.93	1.9072	1.906
△L/L*		1.26%	0.06%	0.0%
M(2)				
−O(3)	1.859	1.85(8)	1.8582(7)	1.857(3)
−O(6)	1.923	1.93(5)	1.9262(9)	1.929(5)
−O(10)	1.852	1.88(2)	1.8642(10)	1.862(4)
Average	1.878	1.89	1.8829	1.883
△L/L*		0.64%	0.26%	0.27%
M(3)				
−O(1)	2.184	2.27(5)	2.2000(8)	2.206(4)
−O(2)	1.927	2.03(2)	1.9563(8)	1.957(4)
−O(4)	1.862	1.90(1)	1.9027(11)	1.907(5)
−O(8)	1.781	1.86(2)	1.8100(12)	1.812(6)
Average	1.978	2.06	2.0042	2.008
△L/L*		4.15%	1.32%	1.52%

* : $\triangle L/L=(L'-L)/L$, where L and L′ are the average bond lengths of clinozoisite and other epidotes.

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Appendix |Fo| -|Fc| Tables

H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)
L=0				L=0				L=1				L=1				L=2			
2	0	54.1503	56.9084	5	6	28.5393	27.9080	7	2	24.7920	26.2544	-1	5	8.4129	9.4525	10	0	16.0565	16.9719
3	0	82.5904	85.5153	7	6	20.6972	21.4361	6	2	8.8348	9.9496	2	5	22.0621	22.5663	12	0	24.0227	24.4544
4	0	73.6563	75.1564	8	6	20.0768	21.1204	5	2	23.7249	22.7398	4	5	10.2493	5.8787	11	1	17.8681	15.0247
5	0	20.3994	20.5566	9	6	28.5642	28.5941	4	2	12.5821	14.0915	5	5	9.9764	11.8281	10	1	17.7192	16.8267
6	0	27.0751	28.2054	7	7	28.5393	28.8437	3	2	19.0097	19.8109	7	5	20.1264	20.4937	9	1	39.5084	39.8368
10	0	29.9539	30.1197	5	7	23.2534	26.6905	2	2	81.2999	81.8591	9	6	22.5833	22.7849	8	1	13.8230	10.5376
11	0	11.9121	8.3181	3	7	10.8201	11.8899	0	2	11.5128	11.7800	7	6	17.7192	17.0490	7	1	14.9894	17.7136
12	1	21.8388	18.5221	0	8	86.2881	90.5903	-1	2	11.6639	10.1248	5	6	9.5545	10.7307	6	1	15.3864	13.4711
11	1	15.9820	14.7620	2	8	16.0565	14.7776	-2	2	39.8558	37.8579	3	6	12.6069	9.9704	5	1	15.6842	14.4644
10	1	11.6143	11.8827	3	8	26.4547	26.2444	-3	2	38.1434	36.1641	2	6	32.8575	32.3601	4	1	67.1047	66.9239
8	1	25.2387	26.4174	4	8	22.6826	24.2761	-4	2	22.3351	22.2082	-2	6	15.1383	12.6000	3	1	42.0893	41.0686
7	1	60.2800	62.6795					-5	2	21.8140	22.1128	-3	6	12.5573	17.3828	2	1	19.8783	20.0911
6	1	11.0931	11.1917	L=1				-6	2	40.1536	41.7342	-4	6	11.4654	10.6917	-1	1	10.4727	11.2189
5	1	55.4408	55.8640	12	0	11.5150	8.0557	-7	2	21.5658	22.3307	-5	6	14.0463	13.5053	-3	1	15.7339	17.8393
4	1	12.9296	10.2819	10	0	15.6346	13.1265	-8	2	11.5150	11.8137	-6	6	22.0125	21.2253	-4	1	25.4869	24.0087
3	1	11.7632	13.5589	9	0	41.9653	43.7490	-10	2	31.1451	32.6572	-7	6	16.2550	15.3675	-5	1	44.6703	44.1921
1	1	10.8946	8.7551	8	0	11.2172	12.2761	-12	2	19.8783	20.6192	-8	6	11.6887	8.8148	-6	1	24.1964	22.1751
0	2	109.5663	121.6660	7	0	39.5332	39.8166	-10	3	14.8653	16.2365	-10	6	21.1687	22.0958	-7	1	9.4552	9.0953
1	2	60.9749	62.9773	6	0	19.4068	21.1796	-9	3	17.9740	18.6282	-8	7	14.0960	12.2702	-8	1	20.0768	20.5390
3	2	14.9397	15.7440	5	0	12.5325	9.5886	-7	3	18.0170	18.5308	-7	7	16.0317	15.9045	-9	1	20.5980	18.8352
4	2	45.4644	47.1132	4	0	17.4958	16.0204	-6	3	25.9336	25.7101	-6	7	16.3295	12.5813	-10	1	21.0198	22.4573
5	2	45.9856	47.9927	2	0	59.9326	60.1582	-5	3	82.3422	83.5554	-5	7	44.5462	46.5979	-12	1	10.9690	9.9448
6	2	13.0040	12.6031	-3	0	21.8140	20.4324	-4	3	8.3136	7.5752	-4	7	11.0435	4.8659	-13	1	13.9719	13.0825
7	2	34.2224	35.6432	-4	0	98.3491	97.5878	-3	3	77.3292	77.5351	-3	7	39.8806	38.3755	-13	2	15.9572	18.4075
8	2	29.8298	29.5517	-6	0	13.2274	12.7342	-2	3	44.4717	45.0069	-2	7	16.6521	19.4073	-12	2	12.8055	15.2139
9	2	41.2207	43.4249	-7	0	13.5252	15.4748	-1	3	9.2815	7.7671	1	7	13.9222	11.9132	-10	2	21.0447	19.8973
10	2	13.3763	15.9640	-8	0	51.8175	53.3041	1	3	24.8168	24.3512	2	7	13.4011	16.6283	-9	2	23.3030	23.5181
11	2	15.5602	16.8208	-9	0	9.3808	2.6207	2	3	34.8428	34.8482	5	7	11.9121	15.8501	-8	2	22.3103	21.1793
12	3	17.2477	18.6341	-10	0	51.9416	54.5317	4	3	11.2420	11.5394	7	7	16.4287	16.9432	-7	2	21.5162	20.1958
11	3	16.1557	16.2789	-12	0	27.3978	27.5201	5	3	24.4198	24.7812	2	8	16.7515	19.0532	-6	2	64.8464	64.6262
8	3	23.4271	21.3638	-13	0	24.0971	25.7776	7	3	30.4999	28.8439	-4	8	25.7847	23.8449	-5	2	27.1744	27.6204
7	3	51.8423	51.7910	-12	1	15.2127	13.2476	8	3	15.8083	16.7932					-4	2	33.8750	32.6418
5	3	47.7972	47.6980	-10	1	14.6419	16.7796	10	3	12.1354	8.8681	L=2				-3	2	29.9787	30.5469
3	3	18.1411	18.0841	-8	1	21.4665	19.9160	10	4	11.4654	10.2593	-12	0	20.2505	18.0785	-2	2	62.3398	61.4297
1	3	20.9206	21.2842	-7	1	12.9544	12.7320	9	4	35.9844	35.1249	-11	0	23.9234	26.5417	-1	2	55.5152	54.1201
0	4	190.0969	210.0326	-6	1	31.7655	31.8377	8	4	12.7558	9.4219	-10	0	9.0581	9.6784	0	2	77.7759	79.3791
1	4	10.9442	11.7319	-5	1	90.6806	93.5321	7	4	29.9043	30.1599	-9	0	29.5072	29.8137	1	2	10.0508	9.9515
2	4	31.0707	30.8203	-3	1	94.8996	96.2323	6	4	9.4304	13.7247	-8	0	54.9444	55.3705	2	2	68.6433	67.3194
3	4	54.6714	56.0645	-2	1	60.7764	61.3885	3	4	9.6537	9.2951	-6	0	19.7045	19.3471	3	2	54.2248	53.1301
4	4	45.6381	46.5577	-1	1	11.2172	12.8205	2	4	36.3070	35.7289	-5	0	67.3529	68.4529	4	2	118.7733	124.4805
5	4	12.8055	15.4466	0	1	11.3165	10.3732	-3	4	13.2770	12.9388	-4	0	27.0503	25.9915	5	2	19.2082	19.1371
6	4	22.9059	22.3942	1	1	24.7175	24.6972	-4	4	50.8745	50.3431	-3	0	76.9570	77.6365	6	2	8.0903	7.8001
10	4	20.2505	22.8679	2	1	47.5738	47.7068	-7	4	10.7953	11.5246	-2	0	50.6511	53.3492	7	2	50.2789	47.7756
8	5	15.8828	18.8521	4	1	12.1354	11.7855	-8	4	39.2850	39.5758	-1	0	54.7707	54.1023	8	2	34.9421	35.7558
7	5	45.2659	44.9380	5	1	21.8140	21.8676	-10	4	43.6032	44.3374	1	0	53.2321	51.7635	10	2	22.5089	22.7220
6	5	14.9397	7.4110	7	1	29.7305	32.2340	-8	5	13.2522	14.1492	2	0	87.5041	89.4782	11	2	18.1659	20.2682
5	5	34.9669	34.8917	8	1	14.3689	17.8332	-6	5	18.2404	17.7556	3	0	23.7001	21.6330	11	3	16.8010	13.0366
0	6	55.3415	54.1196	12	1	15.8331	15.1376	-5	5	51.9416	52.2829	5	0	64.3464	65.3871	10	3	11.8128	14.4715
1	6	30.8225	30.5779	12	2	27.2489	25.7032	-4	5	10.4479	5.6753	6	0	17.3718	17.0967	9	3	33.2545	33.0420
2	6	23.2782	23.3411	9	2	33.7509	34.0615	-3	5	50.9489	48.9910	8	0	35.7289	35.5394	8	3	9.9267	8.3638
4	6	25.1146	23.7225	8	2	17.6448	18.0610	-2	5	27.1000	27.8114	9	0	26.6284	27.1837	7	3	13.1033	10.5632

Appendix |Fo| - |Fc| Tables (continued)

H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)
L=2				L=2				L=3								L=4			
5	3	15.3616	18.2062	-1	6	27.7452	27.7322	5	1	12.1106	9.8115	-10	5	10.0508	10.8906	-2	0	10.7953	11.3648
4	3	52.5620	51.7374	0	6	39.6573	41.3533	7	1	22.5585	22.9560	-7	5	8.7603	2.8357	-1	0	46.0600	47.0305
3	3	20.6476	21.6472	2	6	34.9669	34.1651	8	1	16.4784	14.1555	-5	5	18.3148	19.0396	0	0	19.5308	15.2550
2	3	18.2404	17.2973	3	6	32.3115	30.7351	9	1	10.9690	6.3919	-3	5	58.3443	58.2080	1	0	32.5349	31.6532
-1	3	13.4011	15.1631	4	6	66.7324	67.3021	11	1	18.9104	17.0292	-2	5	18.8111	15.7269	2	0	39.6573	38.8923
-3	3	28.0926	27.4444	6	6	11.2172	5.1298	11	2	36.3092	35.2894	-1	5	76.2869	78.5557	3	0	50.3037	50.5305
-4	3	13.0040	11.8316	7	6	32.1130	31.1438	10	2	15.9820	12.3229	0	5	43.1068	45.2872	4	0	55.0437	55.2329
-5	3	42.6601	42.5950	8	6	25.1643	24.6194	8	2	10.6216	11.4603	1	5	28.7131	26.8047	6	0	20.0023	20.6496
-6	3	20.0520	20.1733	5	7	14.2697	11.8006	7	2	28.1423	29.2380	2	5	25.0402	24.6657	7	0	49.0877	50.0399
-8	3	15.0390	16.7206	4	7	25.8343	25.2129	6	2	35.4881	35.2813	3	5	11.8128	11.4406	8	0	11.7135	11.5915
-9	3	15.9572	16.4965	2	7	13.7982	10.6597	4	2	77.7759	75.8269	7	5	17.6199	17.1043	9	0	14.7660	10.9629
-10	3	20.2009	19.6387	-1	7	11.1924	9.9093	3	2	32.8327	32.3986	7	6	17.7192	18.3700	10	0	16.6273	16.5890
-11	3	12.0113	8.8019	-3	7	18.5622	19.0742	1	2	23.3030	21.6162	6	6	20.6724	22.9443	11	0	21.7892	21.3640
-12	3	13.0288	9.7697	-5	7	24.9161	23.5259	0	2	76.7584	72.6388	4	6	44.4221	45.2909	10	1	12.7558	10.7715
-12	4	14.4434	15.4805	-6	8	11.1179	6.0779	-1	2	46.5812	44.1829	3	6	17.9922	16.6094	9	1	11.3909	11.4373
-11	4	23.2534	21.6229	-5	8	15.5850	18.3259	-2	2	82.1933	79.2856	2	6	8.8844	4.3789	8	1	40.8237	41.5233
-10	4	11.1676	7.8980	-3	8	25.8095	22.8121	-3	2	24.4694	23.5456	0	6	22.3848	22.9452	6	1	31.1947	30.9015
-9	4	23.5263	23.6014	-2	8	12.3340	11.6886	-4	2	21.1687	19.5587	-1	6	16.8506	16.0691	5	1	10.2245	11.7373
-8	4	42.4368	42.0562	-1	8	11.1924	14.1119	-5	2	7.1969	5.9268	-2	6	23.8986	24.1912	4	1	15.3616	14.5873
-6	4	14.2200	12.9084	1	8	17.7440	13.3716	-6	2	45.6133	45.9003	-3	6	8.7603	12.7327	2	1	36.4559	36.4688
-5	4	42.8090	42.4022	2	8	36.4311	35.3236	-7	2	44.4965	45.4374	-5	6	12.5325	6.3642	1	1	47.7476	47.1351
-3	4	47.5490	48.7040	5	8	27.8197	25.5918	-8	2	54.0510	53.0326	-6	6	28.8868	29.5314	0	1	29.5072	27.5127
-2	4	29.3335	29.6369					-10	2	11.1179	13.3811	-7	6	28.7379	26.6353	-1	1	26.1569	25.0054
-1	4	30.3510	30.7307	L=3				-13	2	13.0785	11.1162	-8	6	33.8998	33.9872	-2	1	29.8298	27.5488
1	4	28.3656	29.1912	11	0	30.5495	27.0543	-11	3	9.6289	8.0911	-10	6	11.3909	9.0157	-5	1	18.8856	18.8904
2	4	68.0229	69.0801	7	0	36.7785	36.3787	-10	3	17.2229	16.9641	-5	7	11.9121	10.3345	-6	1	16.9251	16.0860
3	4	12.7062	13.9295	6	0	35.8603	36.1585	-6	3	9.8275	6.5108	-3	7	31.8896	31.2936	-7	1	21.8140	20.4443
4	4	10.7209	8.8941	4	0	53.1824	53.5824	-5	3	20.5980	21.8266	-1	7	40.0295	41.2480	-8	1	15.5105	15.7831
5	4	49.0629	48.7392	3	0	18.7367	18.2435	-3	3	62.1413	62.5453	0	7	30.4006	28.7336	-10	1	20.1761	19.1312
6	4	12.1354	9.5517	2	0	80.3817	75.2283	-2	3	19.0097	18.4777	2	7	11.5143	14.5219	-11	1	42.6601	44.6567
8	4	29.0853	27.5251	1	0	10.8698	10.9237	-1	3	88.2486	88.9885	3	7	10.8201	13.4510	-12	1	12.7062	15.0832
9	4	19.4564	22.1278	0	0	34.9173	34.2451	0	3	59.3618	58.5910	6	7	14.5916	2.3163	-13	1	37.7960	36.2897
9	5	31.9689	31.5226	-1	0	9.1078	9.0486	1	3	20.6476	19.7844	4	8	22.5585	22.2095	-12	2	14.1704	14.4250
7	5	19.2082	17.1252	-2	0	20.0520	19.1213	2	3	27.8941	27.7513	3	8	15.3886	8.8665	-11	2	13.7485	13.9371
4	5	37.4486	38.2302	-4	0	40.2281	38.7728	3	3	21.8884	21.6594	2	8	19.3075	15.3762	-10	2	11.9121	12.1415
3	5	22.1118	20.0398	-5	0	25.0550	24.4693	7	3	17.4710	17.0201	1	8	12.1106	4.2047	-8	2	60.0815	59.2681
2	5	12.7062	14.2984	-6	0	40.6996	41.3777	8	3	12.2039	10.8552	-4	8	15.2375	7.2907	-6	2	59.2626	58.5276
-3	5	10.9939	10.4807	-7	0	27.3730	28.6280	7	4	27.5715	26.1214	-5	8	16.1061	5.9426	-5	2	96.5871	99.5987
-5	5	20.1513	20.2824	-8	0	74.0038	74.2426	6	4	26.0577	26.8693	-6	8	12.7607	18.9011	-4	2	94.9492	97.3104
-6	5	9.5793	10.9135	-9	0	23.8738	22.9270	4	4	37.9201	40.1101					-2	2	83.8312	82.4797
-7	5	11.8376	8.5182	-10	0	40.5011	40.7957	3	4	14.9397	12.8472	L=4				-1	2	52.7854	51.5115
-8	5	17.7937	16.4648	-11	0	22.1614	21.0141	2	4	35.5129	36.4522	-14	0	10.5464	12.5796	0	2	35.9099	35.2009
-9	5	16.1806	13.6848	-13	1	13.7237	5.6529	1	4	9.3559	5.0523	-13	0	34.7684	34.4133	1	2	72.7133	70.9876
-10	5	17.3718	17.0958	-11	1	11.7880	13.9390	0	4	15.2127	16.3471	-12	0	9.5611	13.3838	2	2	57.5502	57.7626
-10	6	14.6171	13.5608	-10	1	17.8433	18.0969	-4	4	18.1907	18.4727	-11	0	11.4496	10.4872	3	2	8.2144	11.1453
-9	6	11.3413	14.4924	-5	1	30.9466	30.7358	-5	4	10.6216	11.0628	-10	0	31.3188	31.5321	4	2	20.8709	21.3839
-8	6	13.0288	12.4036	-3	1	85.6428	87.4947	-6	4	32.6837	32.1283	-9	0	45.9559	47.4044	5	2	37.6471	35.7160
-7	6	12.0610	12.2048	-2	1	24.3701	24.8783	-7	4	19.2330	19.4303	-8	0	11.5895	10.8799	6	2	19.3819	19.8437
-6	6	35.8355	34.2413	-1	1	132.5963	133.7845	-8	4	54.2992	55.9984	-7	0	30.3758	31.1016	8	2	33.1504	29.7643
-5	6	16.6769	18.6301	0	1	77.8008	77.9973	-9	4	15.8331	17.6717	-6	0	85.8062	85.8455	9	2	10.2742	10.6621
-4	6	18.9849	17.9424	1	1	37.9697	36.5899	-10	4	28.9364	31.7470	-5	0	18.7615	18.7946	10	2	11.6391	12.3809
-3	6	12.1602	9.8432	2	1	36.8530	35.4785	-11	4	16.7513	16.9249	-4	0	22.4344	22.1139	10	3	17.0243	11.1186
-2	6	26.1073	26.7672	3	1	19.5556	19.8415	-11	5	11.4902	12.5631	-3	0	16.8506	20.0767	8	3	37.0267	37.3477

Appendix |Fo| - |Fc| Tables (continued)

H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)
L=4				L=4				L=5				L=5				L=6			
6	3	28.5642	26.9653	2	6	31.7159	29.5260	5	1	25.5613	26.7565	1	5	40.5755	41.3474	3	1	34.7435	34.8250
2	3	32.9319	30.9707	5	6	21.0943	20.3942	7	1	12.1196	15.5275	2	5	34.4706	35.7195	2	1	22.4096	21.3074
1	3	43.3550	43.4701	6	6	13.8478	10.9817	9	1	16.5528	12.7486	3	5	10.8698	7.0389	0	1	8.1896	6.3751
0	3	15.6842	15.6154	7	6	13.9726	7.5353	9	2	17.1491	16.6884	4	5	23.2534	22.3171	-1	1	19.5805	19.6373
-1	3	7.6932	9.5488	6	7	18.1411	16.4658	8	2	9.8523	14.2744	5	5	24.3949	21.4263	-2	1	29.0179	28.6520
-2	3	16.5032	16.1399	2	7	14.8156	15.9743	6	2	10.7209	8.4392	7	5	16.6273	14.5079	-4	1	9.9019	5.6450
-5	3	13.3763	8.4696	1	7	22.0621	23.5551	4	2	31.1203	31.4273	4	6	18.4885	18.2344	-5	1	15.7339	14.9207
-6	3	14.1456	15.2475	0	7	10.0259	3.4625	3	2	32.0137	31.2894	3	6	20.9950	19.6181	-6	1	24.0475	23.6241
-7	3	13.6741	10.6454	-6	7	15.9572	9.2603	2	2	26.8022	27.1464	2	6	12.1106	15.3565	-7	1	32.3115	32.4767
-8	3	15.3616	12.4619	-6	8	37.3245	35.9118	1	2	16.2798	14.2180	-4	6	21.3425	20.9563	-8	1	41.0222	41.5583
-10	3	18.3148	17.5002	-4	8	11.6639	9.4246	-2	2	18.4389	17.1077	-6	6	44.0499	43.5190	-9	1	46.8790	48.0323
-11	3	38.9872	38.7214	-3	8	10.5472	12.6063	-3	2	12.8551	12.0167	-9	7	15.4361	9.4452	-11	1	38.6150	37.9035
-12	3	17.7937	14.2938	-1	8	14.8901	15.4589	-4	2	45.1666	43.6654	-8	7	9.9764	5.7235	-13	2	19.7045	21.5421
-13	3	32.4852	33.1273	0	8	12.1354	4.9634	-5	2	79.9846	82.3991	-4	7	24.4446	25.9413	-10	2	37.0515	38.4246
-12	4	15.2127	10.9148	1	8	15.6098	12.0739	-11	2	15.9820	16.1106	-3	7	12.9047	8.1340	-9	2	12.1354	12.2213
-11	4	11.9865	8.2632	2	8	13.3515	9.9276	-11	3	19.7045	20.0305	-2	7	10.6216	6.1266	-8	2	9.0085	10.5418
-10	4	27.1000	26.2120	3	8	22.0125	23.1510	-10	3	12.4580	15.8198	-1	7	10.7209	13.2620	-7	2	28.4153	28.8015
-9	4	37.3741	37.7862					-9	3	14.1704	13.2645	0	7	18.8608	16.3955	-6	2	38.2675	37.5443
-7	4	24.3701	23.7936	L=5				-8	3	8.7603	12.9350	1	7	29.4327	31.4539	-5	2	34.2224	34.3736
-6	4	65.6405	66.3600	9	0	25.7847	25.0546	-4	3	49.7329	49.7586	2	7	28.6138	27.9292	-4	2	34.9917	36.1286
-5	4	14.8405	13.9455	8	0	40.9725	40.6160	-3	3	13.1777	13.8035	3	7	16.9003	14.2078	-3	2	87.1071	87.6937
-4	4	12.4829	14.0462	7	0	25.2635	23.9534	-1	3	31.4181	30.0624	4	7	19.0593	20.0332	-2	2	66.2361	65.7638
-3	4	28.4401	26.4363	6	0	27.8445	27.1807	0	3	29.9539	29.4987	1	8	17.7440	18.3947	-1	2	20.0023	19.5249
-1	4	32.1130	32.9409	5	0	27.4226	28.5921	1	3	60.7764	59.8918	-1	8	10.8201	13.3196	0	2	60.4041	60.6712
0	4	8.1647	5.7284	3	0	60.2890	60.6067	2	3	52.1898	51.4710	-3	8	16.5280	13.8301	1	2	34.1728	34.0789
1	4	18.9849	19.1848	1	0	44.6455	44.2179	3	3	16.4287	17.9582	-6	8	13.0040	14.3967	2	2	23.1541	23.6396
2	4	22.9804	23.2735	0	0	10.3982	11.4961	4	3	31.5911	32.2291					3	2	51.9912	54.7356
3	4	39.3347	39.6044	-1	0	37.9946	36.7811	5	3	18.1659	17.9360	L=6				4	2	16.1806	15.7704
4	4	40.6003	41.1126	-2	0	23.1293	23.4282	7	3	12.5821	10.0816	-14	0	18.8360	18.2079	7	2	20.4242	20.9268
5	4	8.9341	4.3975	-3	0	47.2760	46.1734	9	3	12.7558	10.3038	-13	0	13.4755	6.2110	8	3	16.6521	17.0948
6	4	12.7062	16.0952	-4	0	17.5951	17.1870	9	4	20.6228	20.3546	-11	0	14.2449	13.6357	7	3	14.0215	18.0655
7	4	39.1609	39.9928	-5	0	18.1659	19.9964	8	4	32.8078	33.5294	-10	0	23.6256	23.7386	6	3	18.2155	19.6897
8	4	12.7558	10.2094	-6	0	35.0910	35.2247	7	4	17.4462	19.2785	-9	0	36.7537	35.0849	5	3	18.7119	18.9512
9	4	10.8698	8.3565	-7	0	14.7650	15.0566	6	4	21.1936	21.2596	-8	0	13.3018	12.0003	4	3	25.7350	25.5259
8	5	32.3363	30.8848	-8	0	28.0182	30.7975	5	4	18.3644	22.0612	-5	0	38.4909	38.4836	3	3	33.1056	31.4895
6	5	22.3351	23.3764	-9	0	10.0508	10.4605	3	4	44.3228	43.7936	-4	0	126.6154	132.9214	2	3	19.7294	20.0639
5	5	12.3340	10.2242	-10	0	21.2630	21.1504	1	4	31.7159	31.3543	-3	0	70.3805	68.5025	1	3	14.2945	10.9957
4	5	9.6537	10.5834	-11	0	23.7993	23.9866	-1	4	21.1936	21.8819	-2	0	64.4741	62.7563	-1	3	9.7778	8.9112
2	5	22.7818	21.7211	-14	0	16.5776	13.4010	-3	4	25.9584	25.9980	-1	0	118.4011	119.1353	-2	3	24.4942	23.6100
1	5	21.1936	19.8582	-12	1	13.2274	6.2620	-5	4	10.7705	12.3046	0	0	36.1829	35.7462	-3	3	10.1004	9.0323
-2	5	12.6814	11.6260	-11	1	22.0125	23.1868	-6	4	25.4547	26.6256	1	0	13.5500	12.3724	-6	3	18.6871	19.7344
-5	5	12.9792	11.2799	-10	1	19.6301	19.0331	-7	4	12.3610	11.6826	2	0	55.5649	56.3299	-7	3	26.5540	26.5516
-7	5	14.7711	15.4623	-9	1	12.1602	12.4927	-8	4	21.0943	21.7799	4	0	27.0751	27.9360	-8	3	34.6939	35.9031
-10	5	10.6216	12.3323	-8	1	15.9324	16.2612	-9	4	11.8624	8.2846	5	0	38.0938	36.6775	-9	3	39.0368	38.9940
-11	5	32.6341	35.0135	-5	1	13.8974	11.8991	-10	4	15.9572	16.9243	6	0	44.1491	41.9077	-10	3	12.1106	9.5301
-8	6	35.7859	35.7205	-4	1	63.6800	63.2607	-11	4	18.3893	19.3643	8	0	19.6053	19.1240	-11	3	31.4925	29.8453
-6	6	31.7407	32.4313	-3	1	8.5618	9.9355	-11	5	20.6724	17.6041	9	0	19.3819	21.1116	-10	4	20.1761	18.5242
-5	6	53.5029	55.1748	-1	1	42.4864	41.3552	-10	5	15.8083	13.5205	9	1	11.7457	2.6968	-9	4	25.5365	27.3969
-4	6	51.3957	52.1273	0	1	37.0515	36.7234	-8	5	13.3515	11.7658	8	1	16.9003	17.2581	-5	4	30.6488	31.2623
-2	6	40.3047	39.5138	1	1	72.1425	70.8147	-4	5	34.2720	35.0800	7	1	21.0695	17.3715	-4	4	89.4398	90.8055
-1	6	24.1219	23.9606	2	1	62.4639	61.2161	-3	5	10.3486	1.7322	6	1	23.2782	22.9727	-3	4	43.3798	43.3053
0	6	16.5776	17.6820	3	1	13.5748	13.4397	-1	5	26.3803	25.4514	5	1	23.5760	23.3906	-2	4	36.1333	37.9965
1	6	40.2529	41.2771	4	1	35.7289	34.9509	0	5	18.9678	21.6344	4	1	29.5320	28.4058	-1	4	81.1510	83.1025

Appendix |Fo| - |Fc| Tables (continued)

H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)
L=6				L=7				L=7				L=8				L=8			
0	4	22.8563	24.3534	1	0	13.8726	13.6447	3	3	12.0362	10.2115	-9	0	36.6296	36.8771	1	3	21.0447	20.1124
2	4	41.2455	42.1004	0	0	24.8665	23.7765	4	3	18.2404	21.2219	-8	0	18.9601	18.2795	0	3	36.9274	38.8407
4	4	17.8929	20.9552	-1	0	29.6313	30.0387	6	3	10.6712	6.9497	-7	0	48.3928	48.9644	-4	3	10.4975	8.8314
5	4	29.1101	29.3371	-2	0	18.7615	18.2126	7	3	18.7615	21.1641	-6	0	60.0815	60.4109	-5	3	23.9234	24.7775
6	4	32.4852	32.8651	-4	0	16.0565	15.4307	8	3	13.1529	8.7126	-4	0	27.4722	26.1460	-7	3	26.2314	25.4226
7	4	11.5895	6.3364	-5	0	17.3718	17.4361	7	4	17.7440	18.3917	-3	0	81.8955	81.9585	-8	3	12.2843	12.5933
8	4	19.0593	16.8984	-6	0	12.1602	11.6358	6	4	21.3176	20.9783	-2	0	59.6596	59.3835	-9	3	12.7558	12.9186
6	5	15.4609	16.6788	-7	0	13.1033	13.2201	5	4	34.1479	35.7459	-1	0	9.9092	11.7449	-10	3	12.3588	8.7202
5	5	21.9950	18.9999	-8	0	10.8698	9.4929	2	4	30.2269	29.3351	0	0	3.7603	3.9903	-11	3	14.5923	13.4503
4	5	17.3718	19.6290	-9	0	19.5060	17.4097	1	4	15.8230	10.6387	1	0	64.9953	65.5739	-12	3	10.9939	10.4183
3	5	26.4051	24.0411	-11	0	29.2094	25.1180	0	4	18.1163	18.2702	2	0	10.1250	7.4782	-12	4	15.1631	9.7486
2	5	13.8230	12.1908	-12	0	33.8005	32.9213	-1	4	20.6213	21.7309	3	0	14.4186	14.2792	-11	4	10.2990	9.8402
-1	5	15.5353	16.4083	-13	0	19.9775	22.9725	-2	4	9.0333	9.6789	4	0	38.3135	38.3915	-9	4	27.9934	27.4238
-2	5	12.5077	13.0213	-14	0	26.3955	25.9593	-5	4	13.1033	13.0357	6	0	15.1879	19.0937	-8	4	12.1106	12.7799
-3	5	8.5122	3.9991	-11	1	12.9544	14.2518	-6	4	10.7457	8.1901	7	0	21.4169	20.3781	-7	4	38.8880	38.0719
-5	5	10.1749	10.6090	-9	1	24.2460	23.4583	-7	4	9.5545	7.7543	8	1	14.5134	22.9285	-6	4	41.2455	42.5522
-6	5	15.5602	15.1943	-8	1	24.8913	23.9104	-9	4	12.4069	13.5583	8	1	14.0960	15.8222	-4	4	22.4344	21.6446
-7	5	21.8388	22.4442	-7	1	54.6467	56.5384	-11	4	23.9052	22.9138	7	1	15.4609	16.7548	-3	4	57.6991	59.2828
-8	5	28.0926	29.2343	-6	1	66.7076	67.4478	-12	4	29.7912	27.1733	6	1	14.3193	13.4748	-2	4	43.4046	44.2041
-9	5	35.7610	36.3767	-4	1	24.2212	23.4320	-11	5	14.8397	10.0896	5	1	10.7953	10.4107	0	4	10.9442	2.9822
-11	5	29.4079	31.6397	-3	1	31.8152	31.4530	-9	5	13.8974	14.3082	4	1	10.1997	9.6189	1	4	50.4278	50.1590
-10	6	25.8591	25.1101	-2	1	41.8660	39.6555	-8	5	19.8075	17.9902	3	1	32.7334	31.8853	3	4	12.6069	10.2206
-7	6	20.5980	16.8629	0	1	50.9737	50.8006	-7	5	33.9494	34.5416	2	1	29.2054	27.2657	4	4	29.9539	29.9731
-6	6	23.0796	24.5778	1	1	13.3266	14.1217	-6	5	43.1068	43.2802	1	1	20.9702	20.5290	6	4	15.0390	16.1368
-5	6	16.9003	17.3340	2	1	25.2387	25.6194	-4	5	9.6515	13.9505	0	1	43.9010	45.8786	3	5	17.1236	19.1325
-4	6	23.9979	21.7007	3	1	9.3808	7.5370	-3	5	19.2827	16.4186	-4	1	9.6537	8.3642	2	5	17.4452	20.2642
-3	6	48.5665	49.5448	4	1	22.4096	22.3759	-2	5	24.5438	25.7159	-6	1	28.3620	29.2416	1	5	11.5150	12.7942
-2	6	41.0470	41.7836	5	1	13.5500	8.2326	0	5	32.7830	32.8231	-7	1	22.5089	22.6629	3	5	30.3758	30.2889
0	6	29.8050	30.7482	7	1	22.0373	22.1198	1	5	9.7778	13.1320	-8	1	12.2595	14.5547	-6	5	21.5235	19.0115
1	6	21.9877	21.5603	7	2	30.1028	30.4829	2	5	13.9471	17.9429	-9	1	15.4857	11.9607	-7	5	10.4479	10.9055
2	6	10.9442	12.0077	6	2	29.1101	26.5849	4	5	14.1704	15.3271	-10	1	9.0581	10.1032	-5	5	11.4727	10.1594
3	6	32.9567	31.7861	5	2	50.8745	48.9922	5	6	34.5947	33.6996	-11	1	13.5500	15.0732	-9	5	9.9019	5.3548
4	6	10.5472	10.6885	4	2	13.1529	12.7975	4	6	15.5602	9.5082	-12	1	11.1924	11.4286	-11	5	13.2025	12.0835
4	7	15.2623	14.9447	0	2	63.2829	63.2823	2	6	10.7457	3.5006	-13	2	20.0272	17.5937	-10	5	30.8721	29.5521
3	7	19.1586	19.1904	-1	2	13.4507	13.0961	0	6	34.4706	35.1768	-11	2	37.6719	38.4349	-6	6	21.4665	22.7320
2	7	15.0142	12.6749	-2	2	19.2082	19.4991	-1	6	10.9194	8.3709	-10	2	40.7244	43.0038	-5	6	34.7757	32.5940
-2	7	11.7135	12.6750	-3	2	9.8771	12.9586	-2	6	11.3187	10.3503	-8	2	15.5105	16.5024	-4	6	13.0298	13.1735
-6	7	11.8873	11.2373	-5	2	34.1231	31.8122	-5	6	19.4316	17.9733	-6	2	38.1434	37.7069	-3	6	19.8286	21.4318
-8	7	25.4124	21.5039	-9	2	20.1016	19.0720	-9	6	11.8376	12.6542	-5	2	53.8525	52.8948	-2	6	15.7339	9.7748
-6	8	11.6639	2.9589	-11	2	28.1423	29.3500	-8	7	15.4112	13.7171	-4	2	24.1716	23.4438	-1	6	30.9969	31.7068
-5	8	18.5630	19.1322	-12	2	26.1817	27.4183	-7	7	31.0955	31.1925	-3	2	34.4706	34.7122	0	6	26.0040	26.9585
-4	8	45.8119	43.9305	-13	2	27.8197	25.2330	-6	7	35.8851	32.3802	-2	2	19.1586	19.2526	1	6	26.1817	23.6967
-3	8	20.3746	22.8841	-11	3	13.3018	15.7637	-4	7	14.7412	10.7084	-1	2	48.8643	48.6262	2	6	17.9177	20.1438
-2	8	17.3966	18.4507	-9	3	25.5861	25.1131	-3	7	14.2449	14.7296	0	2	46.5563	45.7890	3	6	29.3583	29.1253
-1	8	39.0368	41.0284	-8	3	21.2680	21.4767	-2	7	20.7220	17.0965	1	2	36.3070	36.4818	4	6	19.1338	10.7431
0	8	13.7733	12.4727	-7	3	52.1898	52.0307	0	7	25.6110	24.9417	2	2	30.8969	30.4907	2	7	17.0491	11.5314
L=7				-6	3	57.7239	58.5274	2	7	16.7513	15.5466	3	2	41.5434	42.0655	0	7	23.9482	22.3793
9	0	10.4727	3.4190	-4	3	20.8213	20.9696	-1	8	13.6741	12.4678	4	2	18.0915	16.4293	-2	7	11.5646	4.9747
7	0	21.6651	21.9359	-3	3	26.6533	28.2657					6	2	24.5686	26.0475	-6	7	13.4755	14.0228
6	0	25.6358	25.8270	-2	3	33.3042	32.4836	L=8				7	2	16.7762	17.7724	-7	7	17.6944	17.7333
5	0	46.0600	45.5717	0	3	44.1243	44.2741	-12	0	14.0463	13.6371	7	3	13.5500	12.9321				
2	0	40.7492	42.7933	2	3	24.2708	24.0045	-11	0	12.8303	11.8529	3	3	29.4824	31.7456				
								-10	0	9.7282	9.5603	2	3	21.3176	22.0581				

Appendix |Fo| -|Fc| Tables (continued)

H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)	H	K	F(obs)	F(calc)
L=9				L=9				L=10				L=10				L=11			
4	0	17.4710	18.2766	1	3	14.0711	14.2374	2	0	34.9173	34.4815	-1	4	40.1536	39.7629	-5	2	10.1004	0.6009
3	0	25.5606	24.5071	2	3	19.4812	19.8548	3	0	23.7993	20.7472	0	4	12.5325	10.0630	-7	2	22.0621	23.7714
2	0	27.9934	29.6339	4	3	16.9995	19.7658	4	0	20.3498	22.0197	1	4	10.5472	10.4430	-8	2	34.7435	35.4451
-1	0	9.0333	10.1091	4	4	16.5776	14.8319	6	0	28.7875	28.5625	2	4	26.2066	28.0362	-9	2	26.3803	26.0991
-2	0	39.8806	39.2369	3	4	17.0740	19.6895	5	1	30.5991	33.1079	3	4	19.7542	16.5517	-13	2	19.5805	14.8460
-3	0	16.6769	16.4044	2	4	23.5015	23.5149	4	1	32.5349	32.2390	4	4	18.0915	18.8568	-12	3	18.0666	15.3251
-6	1	7.9166	7.5933	0	4	8.8348	2.1952	2	1	10.3734	10.5101	-1	5	11.8624	11.0338	-11	3	10.1997	3.9652
-7	0	22.4592	23.2535	-1	4	11.0931	6.6919	-1	1	19.4316	20.4394	-2	5	11.7135	12.4001	-10	3	10.3734	2.5719
-9	0	28.4897	28.1595	-2	4	24.3453	27.0355	-2	1	19.9279	16.8243	-10	5	13.1033	13.5898	-9	3	12.4084	11.2323
-10	0	38.2179	35.5788	-3	4	19.3238	10.4192	-3	1	15.4112	14.1377	-9	6	32.8823	32.4361	-8	3	33.2794	32.4057
-11	0	47.7476	46.3338	-7	4	18.7367	18.6398	-4	1	12.7807	13.5133	-8	6	23.2037	21.7314	-7	3	26.7029	25.7120
-12	0	45.8615	47.0745	-9	4	23.8241	22.5309	-5	1	12.2347	11.6069	-7	6	11.3413	14.9617	-6	3	22.1366	22.4021
-14	0	12.4332	9.8786	-10	4	28.1175	29.4228	-6	1	11.0683	7.0410	-6	6	20.5972	19.0711	-5	3	20.9454	22.0527
-13	1	10.0508	7.4363	-11	4	34.9274	37.6939	-7	1	14.4682	12.7417	-5	6	12.7310	7.4772	-4	3	23.4023	22.6909
-10	1	17.2725	16.5826	-12	4	37.9449	38.3915	-10	1	16.4227	18.8774	-3	6	35.6866	35.8193	-2	3	30.2021	27.4488
-8	1	23.5760	23.8631	-10	5	14.7449	12.0830	-12	1	18.8360	18.0022	1	6	28.5642	30.2491	0	3	24.6679	27.2139
-7	1	14.9397	13.2485	-9	5	9.9764	3.3022	-13	1	10.4727	3.6595	-2	7	14.6419	10.5218	1	3	20.7965	21.4644
-6	1	21.4665	22.2917	-8	5	16.2728	16.1555	-12	2	23.2037	24.1496	-3	7	11.3165	11.7308	2	4	13.1281	10.4860
-5	1	31.1947	31.4808	-7	5	9.7530	10.4515	-9	2	48.2935	48.9290					1	4	20.1515	21.7502
-4	1	70.7776	71.4429	-6	5	14.7412	15.7211	-8	2	34.9421	33.9892					0	4	30.9714	32.1089
-3	1	17.8433	17.8039	-5	5	24.0227	24.7701	-7	2	24.2957	23.4826	L=11				-2	4	9.7034	10.5778
-2	1	36.8033	36.1638	-4	5	48.9636	49.5459	-6	2	29.9291	29.9461	5	0	17.2973	18.3886	-3	4	12.4829	11.3402
-1	1	24.4446	25.0082	-3	5	16.5528	16.2392	-5	2	11.4902	12.8022	4	0	12.9296	12.9059	-4	4	24.1219	22.5783
1	1	14.7265	14.8251	-2	5	26.7277	27.2771	-4	2	10.5472	9.5527	3	0	8.4859	6.1781	-6	4	28.5634	28.2743
2	1	21.2680	20.9489	-1	5	14.1704	14.1746	-3	2	57.1283	56.8905	2	0	11.1428	12.3318	-7	4	11.3661	12.2482
4	1	20.9454	22.2683	1	5	12.4580	9.6757	-2	2	11.1676	9.6220	1	0	26.1569	25.8391	-9	4	17.1236	17.1776
7	1	11.5624	15.5231	2	5	13.4230	13.7459	-1	2	14.3441	11.0111	0	0	38.5653	38.1111	-10	4	12.7310	13.4032
7	2	13.2025	14.0727	4	5	17.0988	17.3627	1	2	44.2732	46.5775	-2	0	12.7310	13.1146	-10	5	10.2493	1.6880
6	2	18.9849	18.3805	3	6	23.1293	21.3196	2	2	26.3058	25.1430	-4	0	28.7675	28.9374	-9	5	15.8083	13.5627
5	2	9.7530	12.0013	2	6	17.2725	15.7098	4	2	33.0312	31.5521	-6	0	35.3143	36.2123	-8	5	27.2737	27.6151
3	2	32.6341	32.1345	1	6	10.5720	11.3208	5	2	16.1557	12.8370	-7	0	17.9433	16.1054	-6	5	20.4972	20.4669
2	2	25.7599	24.5299	-3	6	12.7310	14.3879	6	2	12.6069	4.1921	-9	0	22.1373	20.6344	-5	5	9.6537	12.0340
1	2	15.1631	15.4827	-7	6	19.0345	15.5456	5	3	31.0955	30.9846	-10	0	16.5528	15.1365	-4	5	20.8461	21.6252
0	2	13.5748	9.9368	-9	6	10.9442	15.1474	4	3	27.4474	28.0842	-12	0	14.1456	13.2428	-2	5	20.2505	23.2956
-1	2	9.1574	6.7718	-7	7	11.3909	7.6415	0	3	8.9341	9.1194	-13	1	10.5472	1.4995	0	5	23.6504	21.8647
-2	2	17.6696	18.9076	-5	7	14.4930	12.0856	-1	3	21.5410	22.2855	-12	1	19.8060	17.1392	1	5	18.5382	20.3055
-3	2	27.3730	26.1230	-4	7	36.9522	36.4743	-2	3	13.4259	15.7250	-9	1	14.7660	15.9927	0	6	25.6110	24.9653
-4	2	10.1501	8.8614	-2	7	16.3295	17.1167	-3	3	14.1704	15.9737	-5	1	37.6967	37.1061	-3	6	12.9544	12.8956
-7	2	18.2155	20.1102	-1	7	14.6916	17.0226	-4	3	8.7355	11.2992	-7	1	23.8008	24.1074	-7	6	18.0666	14.9102
-8	2	13.0536	10.6458					-6	3	8.6363	7.5442	-6	1	25.1394	25.9246	-8	6	20.7220	23.7751
-9	2	21.3176	22.7221	L=10				-7	3	12.0362	9.3103	-5	1	19.1834	20.1724				
-10	2	13.4259	11.8957	-11	0	27.5715	27.1519	-10	3	17.9177	16.1883	-4	1	27.6211	27.2021				
-11	2	40.2529	39.0875	-10	0	28.3904	27.7670	-11	3	9.5297	4.0290	-2	1	31.8152	31.7388	L=12			
-12	2	19.3075	21.1071	-9	0	24.3701	24.0527	-12	3	19.0841	17.8725	0	1	28.6138	30.5514	-13	0	23.1045	23.3656
-10	3	15.0142	15.7670	-8	0	9.8523	6.9348	-11	4	24.5190	22.4494	1	1	26.1817	26.4067	-12	0	12.0610	6.3416
-8	3	21.2680	22.1344	-7	0	62.9603	63.4713	-10	4	23.8490	23.1658	2	1	12.2543	9.2713	-10	0	36.4063	34.4426
-7	3	10.4727	11.5627	-6	0	16.0565	13.4063	-9	4	22.6081	19.7523	3	1	11.3165	15.3743	-9	0	19.9031	18.0815
-6	3	21.7892	20.3020	-5	0	29.4824	28.6300	-7	4	51.1475	50.4721	4	1	11.2668	10.5626	-8	1	12.6318	13.4264
-5	3	24.6183	24.3979	-4	0	27.5219	28.5287	-6	4	14.4434	11.3892	5	2	11.0683	5.7179	-7	0	13.3763	15.2191
-4	3	60.6027	61.8025	-3	0	19.6301	19.2794	-5	4	21.3746	21.5857	2	2	16.3295	19.4574	-6	0	10.7209	13.8572
-3	3	11.8128	11.3287	-2	0	67.2040	67.1886	-4	4	22.0373	22.1395	1	2	17.9177	17.2141	-5	0	59.8334	58.2310
-2	3	32.3363	30.3706	-1	0	48.4424	49.0587	-3	4	15.0142	14.9828	0	2	37.1508	36.4284	-4	0	8.3844	2.9655
-1	3	26.9263	25.7562	0	0	12.6566	11.7063	-2	4	51.4701	51.6163	-3	2	19.2404	17.4209	-3	0	10.2990	8.9869

Appendix |Fo|-|Fc| Tables (continued)

H	K	F(obs)	F(calc)
L=12			
-2	0	32.7334	32.3054
0	0	20.6724	20.0196
1	0	36.5552	36.3394
4	0	12.2843	13.3284
2	1	27.6956	27.1294
1	1	27.4226	25.9591
0	1	17.8929	18.2710
-2	1	11.9683	5.2225
-5	1	14.4186	15.1384
-7	1	11.7632	9.5379
-9	1	13.6741	10.9667
-10	1	31.6663	30.6281
-12	1	33.7509	32.8813
-13	1	21.9877	21.4650
-11	2	29.5816	31.8776
-8	2	13.4259	16.0128
-7	2	52.1401	51.9743
-6	2	34.1231	34.6092
-5	2	26.4795	26.3620
-4	2	39.1361	40.6527
-3	2	36.7785	37.6046
-2	2	10.3486	8.3607
-1	2	41.3944	40.8192
1	2	13.3515	11.2605
2	2	27.0007	27.2482
3	2	15.8331	15.1402
2	3	23.5263	24.5905
1	3	21.2184	23.4833
0	3	14.0215	17.4028
-10	3	28.0678	27.0117
-12	3	25.9584	29.0401
-10	4	27.7204	27.3567
-9	4	10.6712	15.3726
-7	4	11.2668	13.3534
-6	4	9.8275	10.5942
-5	4	45.0674	45.6981
-2	4	25.3628	25.6748
0	4	17.1236	15.8412
1	4	28.1423	29.7807
-6	6	23.8241	23.6702
-5	6	19.6797	16.6257
-4	6	27.2737	25.8284
-3	6	28.2167	26.2789
L=13			
2	0	12.8055	12.7681
1	0	22.0125	21.3374
0	0	13.3515	12.6738
-2	0	10.3238	5.0520
-3	0	19.2578	18.9300
-4	0	15.1631	12.7476
-5	0	9.1574	6.4319
-7	0	10.5223	12.2826
-9	0	17.1484	16.0748
-10	0	16.7762	17.1056
-11	0	14.7164	11.0050
-12	0	10.9690	1.3549
-12	1	10.9194	2.2767
-11	1	19.6549	15.2495
-10	1	34.1231	34.7633
-9	1	9.5048	6.1561
-8	1	29.6561	28.9123
-6	1	21.5658	19.4566
-5	1	12.2099	7.7318
-4	1	34.0983	35.0739
-3	1	41.4441	42.8386
-2	1	9.8523	15.0957
-1	1	19.5308	22.6001
1	1	10.5223	12.4512
2	2	30.4006	30.8275
-1	2	14.6916	15.1418
-2	2	20.1761	20.3475
-3	2	25.4124	27.0068
-4	2	28.2167	28.9955
-7	2	10.5720	5.8383
-12	2	15.4857	13.9147
-11	3	17.3221	16.6078
-10	3	27.1744	31.5249
-8	3	25.6358	26.2780
-7	3	13.1777	4.4330
-6	3	18.8360	17.1619
-5	3	11.1676	7.4133
-4	3	31.0955	31.5840
-3	3	34.3217	35.7897
-1	3	15.2623	17.6347
1	3	11.7135	8.6060
0	4	10.9194	9.8629
-2	4	10.2245	3.4774
-3	4	10.1501	14.7144
-7	4	8.9341	10.2571
-8	4	8.8844	7.6084
-9	4	12.6814	13.6470
-10	4	16.1061	14.1092
-8	5	16.1557	21.1278
-6	5	12.3091	15.0442
-4	5	20.7220	23.9388
-3	5	33.1056	34.4176
-2	5	12.6318	10.5885
L=14			
-11	0	17.9177	18.4486
-10	0	19.3075	18.7559
-9	0	22.4344	23.2337
-8	0	30.3013	28.9155
-7	0	35.5625	35.8956
-6	0	13.9471	15.0243
-4	0	16.5578	12.3856
-3	0	32.9071	33.4927
-1	0	10.5223	8.5631
0	0	29.3583	29.4720
1	1	13.1529	11.5683
-1	1	35.6618	35.4863
-3	1	10.1004	9.2143
-4	1	11.1676	6.1142
-7	1	19.7790	19.0278
-10	1	26.1073	24.8365
-11	1	10.2493	10.2511
-10	2	16.3791	15.4421
-9	2	32.9319	34.7049
-8	2	21.3921	22.0962
-6	2	54.1007	56.0854
-5	2	19.4316	19.8422
-2	2	19.9031	23.2645
-1	3	32.7830	33.5512
-2	3	12.4580	11.1708
-3	3	10.5720	8.0184
-4	3	11.0683	7.4754
-5	3	10.2742	5.3298
-7	3	15.6346	14.3064
-10	3	21.3176	22.5923
-8	4	21.8636	23.9458
-7	4	27.3445	29.4012
-6	4	17.3718	12.9024
-4	4	15.7587	10.1685
-3	4	26.7029	27.5418
L=15			
-2	0	10.8201	11.6819
-4	0	19.9279	19.4697
-6	0	13.0288	17.4188
-10	0	20.8958	22.1666
-10	1	11.4654	11.7534
-9	1	15.4857	6.8485
-8	1	15.9572	18.6832
-6	1	29.2094	28.2843
-5	1	11.9624	13.7973
-2	1	13.5252	14.4984
-1	1	12.1851	11.8266
-2	2	18.3148	17.6135
-4	2	10.8946	5.0923
-5	2	11.9617	8.7212
-7	2	10.1253	1.3703
-8	2	13.4989	11.7724
-9	2	12.2099	8.0771
-8	3	16.8258	17.8275
-6	3	23.9730	25.3637
-5	3	12.5551	15.4734
-4	3	11.3413	2.2626
L=16			
-8	0	23.4519	22.2543
-6	0	36.8282	36.6869
-5	0	21.1936	21.4547
-4	0	23.9234	24.1546
-4	1	24.2460	25.9006