Al,Si distribution in a ternary (Ba,K,Na)-feldspar as determined by crystal structure refinement

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Abstract

Refinement of the crystal structure of a ternary barium feldspar with the formula $(Ba_{0.40}K_{0.47}Na_{0.13})(Si_{2.59}Al_{1.41})O_8$, $a = 8.544(2)$, $b = 13.030(2)$, $c = 7.195(2)$Å, $\beta = 115.68(2)°$, space group = $C2/m$ yields a disordered Al,Si distribution, with 0.437 Al in the T_1 site and 0.268 Al in the T_2 site. On the other hand, the lattice parameter c suggests that the investigated specimen probably has a structural state very close to that of maximum order possible for its composition. It is therefore concluded that the state of maximum order for a natural (Ba,K)-feldspar with a Cn (celsian) content of 40 mol% corresponds to a disordered Al/Si distribution. Comparison with the structural data of a Ba-poor feldspar indicates that the disorder shown by such maximum ordered (Ba,K)-feldspars increases with their Cn content.

Introduction

Viswanathan and Kielhorn (1983) have observed that the variations in lattice constants of barium feldspars are similar to those of plagioclases. They concluded that a natural (Ba,K,Na)-feldspar with maximum possible order (as defined by Viswanathan and Brandt, 1980) should exhibit a more disordered distribution with increasing Cn[1] content. In order to prove this statement, Al,Si distributions in natural specimens with different Cn contents are required. The structure of a specimen with the formula $(Ba_{0.19}K_{0.59}Na_{0.22})(Si_{2.82}Al_{1.13}Fe_{0.05})O_8$ has already been reported (Viswanathan and Brandt, 1980). A specimen from Yugoslavia with the chemical formula $(Ba_{0.40}K_{0.47}Na_{0.13})(Si_{2.59}Al_{1.41})O_8$ was chosen for this study.

Experimental and results

The chemical composition was determined by electron microprobe. The crystals were found to be homogeneous and not to contain any unmixed albite or celsian. No attempt was made to determine trace elements such as Sr, Rb *etc*.

The lattice constants determined from a Guinier powder pattern are as follows: $a = 8.544(2)$, $b = 13.030(2)$, $c = 7.195(2)$Å, and $\beta = 115.68(2)°$. The space group is $C2/m$ as determined from precession and Weissenberg photographs. No *b*-split reflections were observed even after 72 hours of exposure.

The crystal chosen for the structure refinement had an approximate size of $0.06 \times 0.18 \times 0.4$ mm. The calculated linear absorption coefficient, μ, is 32.01 cm^{-1}. The procedure adopted to collect and process the data is the same as that described earlier (Viswanathan and Brandt; 1980). Altogether 1367 reflections were used for the final refinement including the unobserved ones (Table 1)[2], and the final residuals, using isotropic and anisotropic temperature factors, were 0.069 and 0.049, respectively. The atomic coordinates (Table 2) and the important bond lengths and angles (Table 3) were taken from the anisotropic refinement. The temperature factor and the r.m.s. equivalents are listed in Table 4.

Discussion

The relevant structural data of the Cn-poor feldspar (Viswanathan and Brandt, 1980) are included in Tables 2, 3 and 4 for comparison. The atomic coordinates of both are almost identical. The mean

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[1] Cn refers to $BaAl_2Si_2O_8$, celsian.

[2] To receive a copy of the observed and calculated structure factors (Table 1), order Document AM-83-214 from the Business Office, Mineralogical Society of America, 2000 Florida Avenue, N.W., Washington, D. C. 20009. Please remit $1.00 in advance for the microfiche.

STRUCTURE FACTORS OF TERNARY BARIUM FELDSPAR (JUGOSLAVIA)
(VISWANATHAN AND KIELHORN)

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
2	0	0	76.2987	79.8586	-79.7764	-3.6233	-3.5599
4	0	0	149.7770	160.4012	160.3679	3.2695	-10.6242
6	0	0	91.4125	89.4067	89.4049	-0.5640	2.0058
8	0	0	3.7642	2.6841	-2.6793	-0.1613	1.0801
1	1	0	5.6238	5.3933	5.3439	-0.7281	0.2305
3	1	0	85.0703	87.9931	87.9516	2.7034	-2.9228
5	1	0	45.8025	44.4016	-44.2844	-3.2243	1.4008
7	1	0	98.5376	100.2298	100.1630	3.6581	-1.6922
0	2	0	17.4517	29.7239	29.4868	3.7472	-12.2722
4	2	0	24.3028	19.5587	-19.4320	2.2229	4.7441
6	2	0	63.9665	63.5379	-63.5219	-1.4237	0.4286
8	2	0	23.8162	21.6326	-21.6275	-0.4705	2.1835
1	3	0	116.6439	123.3324	-123.3262	-1.2297	-6.6885
3	3	0	47.0999	42.5798	42.5480	1.6447	4.5201
5	3	0	96.8244	96.1507	-96.0971	-3.2121	0.6737
7	3	0	21.1782	21.3987	-21.2495	2.5223	-0.2205
2	4	0	9.4384	3.4314	1.3832	-3.1402	6.0070
4	4	0	3.1153	5.7118	5.2640	2.2169	-2.5965
6	4	0	66.0933	68.0015	-67.9896	-1.2673	-1.9081
8	4	0	37.5581	36.3933	36.3933	0.0626	1.1647
1	5	0	20.8826	15.0428	-15.0393	-0.3231	5.8398
3	5	0	72.6684	73.1420	73.1073	2.2503	-0.4735
5	5	0	16.1757	11.2063	10.9859	-2.2114	4.9694
7	5	0	39.4518	39.9066	39.7935	3.0020	-0.4548
2	6	0	18.2449	12.2005	11.8591	-2.8659	6.0444
4	6	0	85.0409	86.2265	86.1849	2.6771	-1.1856
6	6	0	36.4018	35.6187	35.6119	-0.6966	0.7831
8	6	0	32.1955	30.9675	30.9672	0.1413	1.2281
1	7	0	11.0102	6.1922	6.1335	-0.8511	4.8180
3	7	0	37.2122	38.5912	38.5353	2.0772	-1.3790
5	7	0	37.4318	38.5858	-38.4699	-2.9885	-1.1540
7	7	0	54.5110	54.4535	54.3730	2.9601	0.0575
0	8	0	111.5417	115.9436	115.8880	3.5896	-4.4019
4	8	0	14.7347	14.4373	-14.3077	1.9304	0.2974
6	8	0	33.0836	30.9500	-30.9243	-1.2610	2.1336
1	9	0	62.2187	61.1685	-61.1589	-1.0813	1.0502
3	9	0	40.0277	42.9777	42.9333	1.9540	-2.9500
5	9	0	93.0194	95.9306	-95.8778	-3.1822	-2.9112
7	9	0	46.4612	46.5600	46.4762	2.7910	-0.0987
0	10	0	107.2521	112.0327	111.9724	3.6723	-4.7805
2	10	0	28.6878	29.4031	-29.2674	-2.8209	-0.7152
4	10	0	62.6307	63.9217	63.8792	2.3288	-1.2910
6	10	0	4.4920	3.9675	-3.9037	-0.7088	0.5245
1	11	0	0.0000	2.3471	-2.3348	-0.2402	-2.3471
3	11	0	72.0460	74.9171	74.8891	2.0461	-2.8711
5	11	0	9.3971	9.8531	-9.6716	-1.8825	-0.4560
0	12	0	4.2417	5.2536	4.5679	2.5952	-1.0119
2	12	0	13.7556	12.6923	12.5117	-2.1338	1.0632
4	12	0	16.7983	17.3781	17.2882	1.7656	-0.5798
1	13	0	15.8335	15.8672	-15.8510	-0.7161	-0.0337
3	13	0	15.2115	13.9410	-13.9090	0.9446	1.2705

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
5	13	0	7.7141	8.4977	-8.2780	-1.9200	-0.7837
0	14	0	3.8476	2.5834	-1.6578	1.9813	1.2642
2	14	0	53.7978	55.1910	-55.1357	-2.4707	-1.3932
4	14	0	22.8892	23.5779	-23.5502	1.1431	-0.6887
1	15	0	9.4711	9.0525	-9.0387	-0.4996	0.4186
-8	0	1	67.9369	66.9287	66.8884	2.3208	1.0082
-6	0	1	20.9961	17.1450	16.9356	-2.6714	3.8511
-4	0	1	108.2395	108.9893	108.9295	3.6089	-0.7498
-2	0	1	91.3685	83.1198	83.0657	-2.9991	8.2486
0	0	1	17.0713	20.5470	20.3944	2.4989	-3.4756
2	0	1	0.0000	3.7997	-3.6082	-1.1909	-3.7997
4	0	1	8.4563	8.9481	8.9472	-0.1246	-0.4918
6	0	1	34.1954	35.2100	-35.1930	1.0942	-1.0146
8	0	1	0.0000	2.6334	-1.7634	-1.9558	-2.6334
-9	1	1	5.2986	4.6399	-4.1537	-2.0676	0.6588
-7	1	1	18.6356	18.0757	17.9940	1.7169	0.5599
-5	1	1	21.2640	19.6599	19.6543	-0.4667	1.6042
-3	1	1	0.0000	0.8099	0.3275	-0.7407	-0.8099
-1	1	1	8.1610	10.0286	9.7899	2.1752	-1.8676
1	1	1	19.9360	14.7677	14.4498	-3.0475	5.1683
3	1	1	84.0293	86.5962	86.5255	3.4974	-2.5669
5	1	1	49.9606	52.0462	-51.9499	-3.1637	-2.0855
7	1	1	38.3251	37.5634	37.4942	2.2785	0.7617
-8	2	1	6.3233	7.4693	7.2116	1.9449	-1.1460
-6	2	1	100.7536	101.6402	-101.5838	-3.3859	-0.8867
-4	2	1	35.2365	39.7113	39.5458	3.6215	-4.4747
-2	2	1	91.2828	91.5359	-91.4620	-3.6754	-0.2531
0	2	1	47.2209	49.8001	49.7316	2.6112	-2.5792
2	2	1	53.3166	53.6752	-53.6599	-1.2789	-0.3586
4	2	1	19.8818	19.2623	19.2606	-0.2543	0.6195
6	2	1	46.1651	45.3221	45.2931	1.6208	0.8431
8	2	1	21.0052	20.2762	-20.1637	-2.1329	0.7290
-9	3	1	78.0980	76.2599	-76.2054	-2.8821	1.8381
-7	3	1	52.5100	51.6166	51.5810	1.9169	0.8934
-5	3	1	40.8117	39.4234	-39.4110	-0.9907	1.3883
-3	3	1	87.5296	82.9533	-82.9464	-1.0661	4.5763
-1	3	1	86.7689	79.8433	79.8059	2.4457	6.9255
3	3	1	77.0561	82.3680	82.2722	3.9721	-5.3119
5	3	1	91.8506	93.0590	-92.9946	-3.4621	-1.2084
7	3	1	23.0568	22.5712	22.4459	2.3755	0.4856
-8	4	1	33.6001	32.4617	32.3912	2.1384	1.1384
-6	4	1	109.0247	109.9067	-109.8500	-3.5300	-0.8820
-4	4	1	118.6721	121.0224	120.9516	4.1395	-2.3503
-2	4	1	163.9986	165.1032	-165.0542	-4.0229	-1.1045
0	4	1	114.7193	117.7681	117.7322	2.9099	-3.0488
2	4	1	97.3576	98.9303	-98.9218	-1.3007	-1.5727
4	4	1	38.3165	37.6113	-37.6073	-0.5492	0.7051
6	4	1	79.2463	80.4975	80.4736	1.9610	-1.2512
8	4	1	83.4219	81.2496	-81.2078	-2.6059	2.1723
-9	5	1	59.6952	57.7870	-57.7328	-2.5033	1.9082
-7	5	1	69.0081	69.3104	69.2735	2.2618	-0.3022
-5	5	1	16.1832	17.2351	-17.2215	-0.6844	-1.0519
-3	5	1	59.4907	56.2172	-56.2116	-0.7907	3.2735
-1	5	1	96.2907	90.3373	90.2997	2.6063	5.9533
1	5	1	83.9022	93.9254	-93.8565	-3.5980	-10.0233

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
3	5	1	121.6115	128.0483	127.9860	3.9939	-6.4369
5	5	1	75.8109	76.2521	-76.1742	-3.4468	-0.4412
7	5	1	41.9258	40.5630	40.5013	2.2372	1.3628
-8	6	1	57.1949	55.9569	55.9130	2.2150	1.2380
-6	6	1	37.4942	37.6848	-37.5731	-2.8995	-0.1907
-4	6	1	137.0416	140.5933	140.5403	3.8605	-3.5517
-2	6	1	54.7814	57.3639	-57.2652	-3.3636	-2.5825
0	6	1	80.4790	85.6331	85.5921	2.6504	-5.1541
2	6	1	22.8491	24.2878	-24.2609	-1.1418	-1.4387
4	6	1	27.2918	27.8288	-27.8257	-0.4099	-0.5369
6	6	1	33.5978	32.6376	32.6027	1.5090	0.9602
-7	7	1	21.1078	20.7688	20.7130	1.5214	0.3390
-5	7	1	21.7221	21.5525	21.5462	-0.5194	0.1697
-3	7	1	6.9722	4.7979	4.7416	-0.7330	2.1743
-1	7	1	10.9265	13.3981	13.2550	1.9526	-2.4716
1	7	1	3.0273	5.9805	-5.2616	-2.8429	-2.9532
3	7	1	57.2860	61.8090	61.7259	3.2037	-4.5230
5	7	1	56.0330	57.3409	-57.2674	-2.9026	-1.3079
7	7	1	32.9173	32.4194	32.3526	2.0787	0.4979
-8	8	1	6.0589	5.7842	-5.5812	1.5189	0.2747
-6	8	1	54.2597	55.1687	-55.1014	-2.7257	-0.9090
-4	8	1	17.4651	12.8355	-12.5506	2.6894	4.6296
-2	8	1	4.4503	4.2913	-3.2387	-2.8152	0.1591
0	8	1	12.9456	8.4270	-8.1905	1.9825	4.5186
2	8	1	0.0000	2.1489	-1.8738	-1.0521	-2.1489
4	8	1	42.7017	43.3334	43.3334	0.0093	-0.6317
6	8	1	4.6589	5.2874	5.1717	1.1002	-0.6285
-7	9	1	6.2351	4.8804	-4.7466	1.1352	1.3546
-5	9	1	8.6924	8.7573	-8.7410	-0.5335	-0.0649
-3	9	1	18.9017	19.5596	-19.5453	-0.7482	-0.6579
-1	9	1	10.6582	6.1841	-5.9673	1.6230	4.4741
1	9	1	12.9474	16.7900	-16.6066	-2.4748	-3.8426
3	9	1	20.9087	24.5068	24.3515	2.7543	-3.5981
5	9	1	24.9757	26.5379	-26.4215	-2.4828	-1.5621
-6	10	1	18.6541	19.6860	-19.5461	-2.3434	-1.0320
-4	10	1	28.8041	30.7450	30.6090	2.8885	-1.9409
-2	10	1	4.0748	4.4916	-3.6568	-2.6081	-0.4168
0	10	1	14.3658	16.1603	16.0309	2.0415	-1.7945
2	10	1	46.9872	50.6531	-50.6425	-1.0332	-3.6658
4	10	1	4.0006	3.1281	3.1238	-0.1652	0.8725
6	10	1	6.6106	6.1824	-6.0924	1.0509	0.4282
-5	11	1	6.5922	7.7527	-7.7400	-0.4430	-1.1605
-3	11	1	25.3931	25.2009	-25.1941	-0.5827	0.1922
-1	11	1	46.9936	45.3581	45.3154	1.9666	1.6356
1	11	1	48.4461	53.2848	-53.2169	-2.6879	-4.8387
3	11	1	53.5493	55.9140	55.8351	2.9691	-2.3648
5	11	1	40.3851	41.3273	-41.2437	-2.6273	-0.9422
-6	12	1	56.2934	56.3098	-56.2530	-2.5278	-0.0164
-4	12	1	85.2368	85.5408	85.4819	3.1752	-0.3041
-2	12	1	80.4305	80.5711	-80.5173	-2.9438	-0.1405
0	12	1	62.4090	66.0239	65.9873	2.1980	-3.6149
2	12	1	28.5378	29.1096	-29.0945	-0.9377	-0.5718
4	12	1	24.1153	24.6619	-24.6577	-0.4526	-0.5466
-5	13	1	6.2861	6.4771	-6.4400	-0.6931	-0.1910
-3	13	1	22.5185	22.2289	-22.2173	-0.7196	0.2896

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-1	13	1	43.9808	41.3249	41.2852	1.8090	2.6559
1	13	1	55.8639	59.2901	-59.2273	-2.7291	-3.4263
3	13	1	63.9752	65.7413	65.6761	2.9269	-1.7661
-4	14	1	52.9543	53.4842	53.4234	2.5487	-0.5299
-2	14	1	62.2283	62.4965	-62.4409	-2.6350	-0.2681
0	14	1	36.4920	38.9816	38.9395	1.8106	-2.4896
2	14	1	5.9708	5.0238	-4.9623	-0.7833	0.9471
-1	15	1	13.1724	12.5469	12.4739	1.3519	0.6254
1	15	1	14.2941	14.2582	-14.1253	-1.9421	0.0359
-8	0	2	63.0340	62.5354	62.4483	3.2987	0.4986
-6	0	2	179.8938	189.4545	-189.4101	-4.1009	-9.5606
-4	0	2	113.9114	112.2402	112.2114	2.5418	1.6712
-2	0	2	191.4976	189.9018	-189.8931	-1.8276	1.5957
2	0	2	69.9339	71.7621	71.7383	1.8483	-1.8282
4	0	2	163.8207	179.9555	-179.9163	-3.7562	-16.1348
6	0	2	44.9165	44.4091	44.3068	3.0125	0.5074
-9	1	2	14.2054	13.5552	-13.5340	-0.7572	0.6502
-7	1	2	34.6055	35.3509	-35.3391	-0.9114	-0.7454
-5	1	2	60.9024	60.5468	60.5045	2.2634	0.3556
-3	1	2	113.2960	115.3349	-115.2700	-3.8695	-2.0389
1	1	2	88.0060	105.1139	-105.0323	-4.1414	-17.1079
3	1	2	52.8689	55.9769	55.9114	2.7078	-3.1080
5	1	2	40.5588	41.9044	-41.8763	-1.5321	-1.3456
7	1	2	16.4873	15.7161	-15.7143	-0.2391	0.7712
-8	2	2	68.8354	67.9681	67.8843	3.3736	0.8673
-6	2	2	20.5686	21.2920	-21.0843	-2.9670	-0.7234
-4	2	2	131.0767	129.2490	129.2175	2.8550	1.8277
-2	2	2	39.0236	31.9136	31.9011	-0.8935	7.1099
0	2	2	56.5087	55.2702	55.2702	-0.0818	1.2385
2	2	2	105.4330	113.0100	112.9880	2.2280	-7.5769
4	2	2	4.1073	3.6475	-2.6630	-2.4925	0.4598
6	2	2	80.5389	81.0345	80.9663	3.3245	-0.4956
-9	3	2	13.2969	14.4792	14.4783	-0.1617	-1.1823
-7	3	2	32.6531	31.6623	31.6593	-0.4364	0.9909
-5	3	2	26.6455	26.6077	26.5055	2.3297	0.0378
-3	3	2	78.5860	72.9345	-72.8823	-2.7587	5.6515
1	3	2	51.9060	55.4862	-55.4033	-3.0310	-3.5801
3	3	2	41.5168	43.7463	43.6457	2.9644	-2.2294
5	3	2	12.6429	11.3160	11.2669	-1.0536	1.3269
7	3	2	41.5963	41.9529	41.9486	0.5981	-0.3566
-8	4	2	0.0000	2.6503	-0.0792	2.6491	-2.6503
-6	4	2	20.6308	18.4697	18.2878	-2.5858	2.1611
-4	4	2	40.6891	34.7789	-34.7169	2.0757	5.9102
-2	4	2	10.6987	10.8852	-10.8362	-1.0315	-0.1865
0	4	2	9.5325	5.9247	5.9221	-0.1763	3.6077
2	4	2	52.5180	50.6841	-50.6649	1.3938	1.8339
4	4	2	28.4146	26.7774	26.6897	-2.1661	1.6372
6	4	2	0.0000	4.9529	4.2313	2.5745	-4.9529
-9	5	2	15.2767	14.9177	-14.9076	-0.5485	0.3590
-7	5	2	25.0931	26.7605	-26.7423	-0.9876	-1.6674
-5	5	2	38.6696	34.4867	-34.4522	1.5416	4.1829
-3	5	2	60.2507	61.1537	-61.0702	-3.1944	-0.9030
-1	5	2	55.3861	47.4461	47.3508	3.0053	7.9401
1	5	2	67.6620	76.7307	-76.6482	-3.5583	-9.0687
3	5	2	10.0459	5.6214	-5.2175	2.0922	4.4245

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
5	5	2	60.2925	63.3372	-63.3126	-1.7658	-3.0447
7	5	2	6.8888	7.1264	-7.1264	-0.0087	-0.2376
-8	6	2	13.4035	14.1410	13.9026	2.5857	-0.7375
-6	6	2	77.3632	78.6248	-78.5622	-3.1358	-1.2616
-4	6	2	9.6580	12.5257	12.3740	1.9433	-2.8677
-2	6	2	89.8520	81.5044	-81.4914	-1.4566	8.3477
0	6	2	98.0482	95.7604	-95.7575	-0.7448	2.2877
2	6	2	16.4887	13.4819	-13.4226	1.2625	3.0068
4	6	2	63.4836	66.2241	-66.1650	-2.7954	-2.7405
6	6	2	7.0046	4.4858	-3.8168	2.3569	2.5188
-7	7	2	11.5067	10.9940	-10.9763	-0.6245	0.5127
-5	7	2	55.2117	55.0451	55.0023	2.1706	0.1666
-3	7	2	51.4170	50.5266	-50.4309	-3.1086	0.8904
-1	7	2	114.9390	95.1855	95.1086	3.8248	19.7535
1	7	2	49.2891	55.3451	-55.2429	-3.3616	-6.0560
3	7	2	60.5415	63.2138	63.1592	2.6281	-2.6724
5	7	2	17.7355	17.1150	-17.0757	-1.1578	0.6206
-8	8	2	95.8471	95.2108	95.1509	3.3776	0.6363
-6	8	2	51.2346	51.8816	-51.8034	-2.8474	-0.6470
-4	8	2	180.4408	182.6435	182.6191	2.9830	-2.2026
-2	8	2	34.5578	29.0243	29.0158	-0.7014	5.5335
0	8	2	44.9271	41.6127	41.6127	-0.0557	3.3144
4	8	2	29.5068	30.7782	-30.6844	-2.4012	-1.2714
6	8	2	106.6931	108.4320	108.3803	3.3484	-1.7389
-7	9	2	0.0000	1.0888	-0.9769	-0.4808	-1.0888
-5	9	2	73.1794	73.7831	73.7489	2.2473	-0.6037
-3	9	2	84.5190	84.5215	-84.4679	-3.0086	-0.0025
1	9	2	50.2191	56.3447	-56.2567	-3.1484	-6.1256
3	9	2	56.0292	59.4564	59.3985	2.6248	-3.4272
5	9	2	6.9583	6.2875	6.2268	-0.8714	0.6709
-6	10	2	71.1015	70.5628	-70.5034	-2.8940	0.5387
-4	10	2	7.6169	8.3063	8.0870	1.8963	-0.6895
-2	10	2	81.2394	78.4546	-78.4443	-1.2696	2.7848
0	10	2	57.1769	58.7998	-58.7963	-0.6459	-1.6229
2	10	2	8.8592	7.2141	-7.0845	1.3613	1.6452
4	10	2	74.4987	76.6235	-76.5788	-2.6185	-2.1249
-7	11	2	21.1955	20.9912	-20.9743	-0.8410	0.2044
-5	11	2	21.3632	20.6944	-20.6571	1.2430	0.6688
-3	11	2	83.5310	82.9150	-82.8663	-2.8409	0.6160
-1	11	2	28.5135	26.0085	25.8876	2.5053	2.5050
1	11	2	71.9120	80.6298	-80.5704	-3.0943	-8.7178
3	11	2	18.3435	17.8845	-17.8120	1.6082	0.4590
5	11	2	42.2293	43.1416	-43.1172	-1.4514	-0.9123
-6	12	2	3.3099	2.7031	-1.8350	-1.9848	0.6068
-4	12	2	15.3420	14.6644	-14.5967	1.4075	0.6775
-2	12	2	9.1611	8.7402	-8.6964	-0.8739	0.4209
0	12	2	9.8343	10.3558	-10.3521	-0.2789	-0.5215
2	12	2	24.9961	25.3414	-25.3262	0.8764	-0.3453
4	12	2	7.3060	6.3413	6.1087	-1.7018	0.9647
-5	13	2	7.7604	8.1834	8.0495	1.4741	-0.4230
-3	13	2	25.2351	23.5952	23.5397	-1.6174	1.6399
-1	13	2	30.7446	27.4887	27.3752	2.4956	3.2559
1	13	2	8.1129	7.2456	6.9976	-1.8795	0.8673
3	13	2	34.5101	36.5217	36.4678	1.9833	-2.0116
-4	14	2	55.9592	56.5955	56.5674	1.7819	-0.6362

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-2	14	2	36.0185	34.9531	34.9514	-0.3442	1.0654
0	14	2	32.7266	33.7276	33.7271	0.1848	-1.0010
2	14	2	46.1841	50.4646	50.4458	1.3770	-4.2805
-1	15	2	49.5547	42.5095	42.4428	2.3797	7.0452
-10	0	3	54.9203	54.1111	-54.0536	-2.4947	0.8091
-8	0	3	30.5349	30.6327	-30.6009	1.3939	-0.0978
-6	0	3	28.1211	27.4620	-27.4364	-1.1849	0.6591
-4	0	3	118.6501	112.6918	-112.6894	-0.7325	5.9583
-2	0	3	16.3800	11.2546	11.1724	1.3575	5.1255
0	0	3	4.3396	5.6732	-4.9529	-2.7666	-1.3337
2	0	3	12.9775	9.8730	-9.4408	2.8892	3.1045
4	0	3	13.8589	14.0080	13.6895	-2.9702	-0.1491
6	0	3	26.6338	27.4110	27.3146	2.2962	-0.7772
-9	1	3	6.7126	6.7412	6.5560	1.5693	-0.0285
-7	1	3	13.2324	13.5025	-13.2173	-2.7606	-0.2700
-5	1	3	2.7073	5.4999	4.5264	3.1242	-2.7926
-3	1	3	22.6230	25.8388	-25.6170	-3.3787	-3.2158
-1	1	3	102.7550	88.8354	88.7963	2.6359	13.9196
1	1	3	91.6457	98.2544	-98.2396	-1.7067	-6.6087
3	1	3	26.3801	27.3967	27.3958	0.2183	-1.0166
5	1	3	4.3854	4.1246	4.0231	0.9097	0.2608
7	1	3	19.1637	18.0344	-17.9537	-1.7038	1.1293
-10	2	3	10.1805	9.3925	-9.1308	-2.2017	0.7879
-8	2	3	65.5143	65.4374	65.3977	2.2784	0.0769
-6	2	3	33.2596	30.9929	30.9839	-0.7468	2.2667
-4	2	3	31.2823	27.8009	27.8003	-0.1937	3.4813
-2	2	3	54.7012	47.8979	47.8541	2.0479	6.8033
0	2	3	32.1776	34.3544	-34.2377	-2.8299	-2.1768
2	2	3	74.9472	82.2224	82.1449	3.5687	-7.2752
4	2	3	62.7755	66.5802	-66.5055	-3.1533	-3.8047
6	2	3	27.5527	27.9115	27.8099	2.3801	-0.3588
-9	3	3	58.0541	57.1866	57.1452	2.1759	0.8675
-7	3	3	92.8010	94.6632	-94.6187	-2.9040	-1.8622
-5	3	3	143.5044	143.4149	143.3543	4.1709	0.0895
-3	3	3	91.6288	86.4268	-86.3538	-3.5511	5.2020
-1	3	3	56.7981	53.9242	53.8341	3.1157	2.8739
1	3	3	22.8323	18.8887	18.8457	-1.2738	3.9436
3	3	3	11.1043	11.5851	-11.5851	0.0043	-0.4808
5	3	3	51.3611	51.2458	51.2240	1.4962	0.1153
-8	4	3	56.5661	56.1663	56.1171	2.3500	0.3998
-6	4	3	47.8299	46.9300	-46.9160	-1.1458	0.8999
-4	4	3	7.7191	7.1446	7.1306	-0.4461	0.5745
-2	4	3	9.1282	11.3560	11.1527	2.1390	-2.2278
0	4	3	123.6262	125.2335	-125.1871	-3.4112	-1.6074
4	4	3	115.2716	125.1320	-125.0834	-3.4850	-9.8604
6	4	3	39.8955	39.3858	39.3157	2.3477	0.5097
-9	5	3	27.2060	26.8262	26.7782	1.6037	0.3798
-7	5	3	117.5910	119.7353	-119.6871	-3.3975	-2.1442
-5	5	3	101.9667	103.2481	103.1852	3.6029	-1.2814
-3	5	3	129.3832	119.8351	-119.7683	-3.9999	9.5481
-1	5	3	30.2506	29.4498	29.3302	2.6516	0.8007
1	5	3	49.1038	51.1895	-51.1641	-1.6093	-2.0857
3	5	3	54.5527	55.8632	-55.8622	-0.3338	-1.3105
5	5	3	28.3530	28.7318	28.6999	1.3534	-0.3788
-8	6	3	17.2021	17.4119	17.3253	1.7353	-0.2098

H	K	L	Y(OBS)	Y(CALC)	A	B	OBS-CALC
-6	6	3	49.8347	49.5459	-49.5300	-1.2549	0.2888
-4	6	3	66.7580	63.1874	-63.1835	-0.7063	3.5706
-2	6	3	33.2143	29.8778	29.8314	1.6633	3.3365
0	6	3	79.8122	81.5868	-81.5280	-3.0960	-1.7746
2	6	3	65.9890	72.9287	72.8562	3.2499	-6.9397
4	6	3	48.0479	50.4448	-50.3497	-3.0963	-2.3969
6	6	3	30.2318	30.6181	30.5406	2.1771	-0.3864
-9	7	3	17.4662	18.0043	17.9331	1.5999	-0.5381
-7	7	3	6.9630	6.9547	-6.5395	-2.3670	0.0083
-5	7	3	18.3050	20.0759	19.8439	3.0432	-1.7708
-3	7	3	12.8835	14.7316	-14.4344	-2.9441	-1.8481
-1	7	3	102.0487	92.2393	92.2036	2.5667	9.8094
1	7	3	48.9068	53.2251	-53.2068	-1.3961	-4.3183
3	7	3	38.3604	39.8565	39.8557	0.2595	-1.4961
5	7	3	28.4366	29.6149	29.5982	0.9933	-1.1782
-8	8	3	50.0709	50.8293	50.7959	1.8443	-0.7584
-6	8	3	68.1112	67.5343	67.5334	-0.3483	0.5769
-4	8	3	23.5862	21.2687	21.2687	-0.0119	2.3175
-2	8	3	63.1073	56.5501	56.5260	1.6494	6.5572
0	8	3	42.1914	38.0401	37.9898	-1.9566	4.1512
2	8	3	6.7687	8.6770	8.2344	2.7358	-1.9083
4	8	3	0.0000	2.4419	0.4521	-2.3997	-2.4419
-7	9	3	7.2040	5.3821	5.0258	-1.9256	1.8219
-5	9	3	17.3154	18.6899	18.4879	2.7403	-1.3745
-3	9	3	11.4234	7.5471	7.1426	-2.4376	3.8762
-1	9	3	46.6306	43.3242	43.2634	2.2944	3.3064
1	9	3	28.3898	30.6452	-30.6204	-1.2324	-2.2554
3	9	3	29.0898	29.3005	29.2985	0.3480	-0.2108
5	9	3	0.0000	1.4888	-1.3138	0.7005	-1.4888
-6	10	3	28.7698	29.2923	-29.2779	-0.9189	-0.5224
-4	10	3	26.5599	26.3496	-26.3457	-0.4558	0.2103
-2	10	3	43.4209	38.1105	-38.0922	1.1793	5.3104
0	10	3	25.0567	26.8591	-26.7593	-2.3136	-1.8024
2	10	3	25.4503	28.9264	28.8155	2.5305	-3.4761
4	10	3	42.3492	44.2176	-44.1448	-2.5364	-1.8685
-7	11	3	79.9088	80.3674	-80.3235	-2.6555	-0.4586
-5	11	3	39.6844	41.4940	41.4120	2.6073	-1.8096
-3	11	3	78.9142	75.4602	-75.3973	-3.0810	3.4539
-1	11	3	8.4054	6.5337	-6.2425	1.9288	1.8717
1	11	3	31.0677	32.4316	-32.4049	-1.3160	-1.3639
3	11	3	32.2603	34.0759	-34.0753	-0.2040	-1.8157
-6	12	3	31.3173	31.1165	-31.1015	-0.9656	0.2008
-4	12	3	12.1423	11.1883	-11.1793	-0.4494	0.9540
-2	12	3	25.0604	22.6830	22.6314	1.5284	2.3774
0	12	3	72.4707	74.0804	-74.0345	-2.6059	-1.6097
2	12	3	73.6046	80.0640	80.0128	2.8613	-6.4593
-5	13	3	79.9675	79.2797	79.2217	3.0325	0.6878
-3	13	3	45.6801	43.6322	-43.5549	-2.5965	2.0479
-1	13	3	68.8640	63.1438	63.1024	2.2872	5.7202
1	13	3	0.0000	0.9685	-0.4205	-0.8724	-0.9685
-4	14	3	11.2239	9.8860	9.8856	-0.0901	1.3380
-2	14	3	70.9784	63.5969	63.5759	1.6352	7.3815
0	14	3	28.5945	28.6717	-28.6030	-1.9839	-0.0772
-10	0	4	15.9168	15.4371	-15.4146	-0.8337	0.4797
-8	0	4	33.3239	32.4394	32.4389	-0.1720	0.8845

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-6	0	4	112.0317	112.1717	112.1474	2.3325	-0.1400
-4	0	4	53.0726	51.5737	-51.4831	-3.0551	1.4989
0	0	4	12.3411	16.0256	-15.6574	-3.4155	-3.6845
2	0	4	124.4551	135.5068	135.4663	3.3129	-11.0517
4	0	4	32.3032	31.7965	31.7790	-1.0552	0.5067
6	0	4	24.4144	24.8968	24.8927	0.4521	-0.4824
-9	1	4	76.7812	77.6335	77.5629	3.3117	-0.8524
-7	1	4	72.5859	72.0016	-71.9246	-3.3291	0.5843
-5	1	4	105.1822	102.7624	102.7199	2.9577	2.4198
-3	1	4	17.9225	17.6529	-17.5993	-1.3741	0.2696
-1	1	4	24.8854	21.1004	-21.1004	-0.0289	3.7850
1	1	4	88.2929	88.5936	88.5741	1.8571	-0.3007
3	1	4	48.7074	51.0204	-50.9587	-2.5080	-2.3130
5	1	4	73.5078	75.6328	75.5697	3.0877	-2.1250
-10	2	4	16.3018	15.8738	-15.8501	-0.8678	0.4280
-8	2	4	19.1374	19.1161	-19.1087	-0.5296	0.0213
-6	2	4	9.8240	9.0813	-8.9478	1.5519	0.7426
-4	2	4	125.9576	117.2787	-117.2349	-3.2073	8.6789
-2	2	4	37.2319	36.7974	36.6449	3.3458	0.4345
0	2	4	126.2930	127.4460	-127.3894	-3.7970	-1.1530
2	2	4	3.3841	2.5220	0.6365	2.4404	0.8621
4	2	4	59.0430	62.0171	-61.9898	-1.8376	-2.9740
-9	3	4	3.6900	2.8257	-1.4082	2.4498	0.8643
-7	3	4	54.6060	55.6706	-55.5888	-3.0168	-1.0646
-5	3	4	10.3080	13.2059	13.0337	2.1056	-2.8979
-3	3	4	60.6058	54.2431	-54.2161	-1.7128	6.3627
-1	3	4	37.3349	32.5489	-32.5482	-0.2114	4.7860
1	3	4	42.3011	40.3385	-40.3315	0.7512	1.9626
3	3	4	32.5882	35.1656	-35.0862	-2.3624	-2.5774
5	3	4	12.5689	12.2056	-12.0278	2.0759	0.3633
-8	4	4	11.4469	12.3957	-12.3896	-0.3899	-0.9468
-6	4	4	17.2273	16.7443	-16.6877	1.3756	0.4830
-4	4	4	20.8701	23.0636	-22.9341	-2.4407	-2.1935
-2	4	4	10.1394	5.6740	4.8538	2.9384	4.4654
0	4	4	27.4604	30.5017	-30.3469	-3.0694	-3.0413
2	4	4	9.3929	8.3376	7.9698	2.4490	1.0553
4	4	4	41.3909	43.1892	-43.1558	-1.6976	-1.7982
-9	5	4	12.3094	13.7433	13.5055	2.5454	-1.4339
-7	5	4	6.2676	5.7610	5.2450	-2.3831	0.5066
-5	5	4	43.1357	44.3006	44.2329	2.4469	-1.1649
-3	5	4	23.5253	24.6828	-24.6574	-1.1213	-1.1575
-1	5	4	37.0688	31.3993	31.3959	0.4637	5.6695
1	5	4	0.0000	1.2498	-0.0395	1.2491	-1.2498
3	5	4	29.4734	30.3856	30.3471	-1.5289	-0.9121
5	5	4	36.8421	39.1020	39.0181	2.5598	-2.2599
-8	6	4	16.9934	16.4905	16.4894	-0.1384	0.5029
-6	6	4	56.5585	56.9691	56.9415	1.7736	-0.4106
-4	6	4	3.4584	5.7078	-5.2076	-2.3364	-2.2493
-2	6	4	127.0151	113.3885	113.3345	3.4998	13.6266
0	6	4	27.3299	24.0047	23.8453	-2.7618	3.3252
2	6	4	70.0305	74.2273	74.1744	2.8016	-4.1968
4	6	4	9.1005	8.9675	8.8914	-1.1661	0.1330
-9	7	4	43.7568	44.5843	44.4998	2.7435	-0.8275
-7	7	4	52.0387	52.8322	-52.7476	-2.9880	-0.7935
-5	7	4	69.7735	69.9998	69.9574	2.4344	-0.2263

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-3	7	4	20.4955	19.7259	-19.6775	-1.3806	0.7696
-1	7	4	6.9496	6.0546	-6.0530	-0.1385	0.8950
1	7	4	51.3004	53.4249	53.4069	1.3849	-2.1245
3	7	4	42.5649	45.5599	-45.5001	-2.3334	-2.9950
-8	8	4	14.2101	13.1170	-13.1067	-0.5192	1.0932
-6	8	4	10.7884	10.7385	10.6351	1.4867	0.0499
-4	8	4	139.7895	134.2237	-134.1842	-3.2577	5.5658
-2	8	4	68.6375	62.3841	62.3024	3.1916	6.2535
0	8	4	135.9546	138.0244	-137.9745	-3.7132	-2.0698
2	8	4	8.3955	5.7163	5.3183	2.0956	2.6793
4	8	4	50.9684	52.6607	-52.6358	-1.6221	-1.6923
-7	9	4	85.9132	86.1256	-86.0707	-3.0733	-0.2124
-5	9	4	51.5001	50.3638	50.3123	2.2771	1.1363
-3	9	4	33.8741	31.2703	-31.2386	-1.4075	2.6038
-1	9	4	64.4728	61.3486	-61.3472	-0.4247	3.1241
1	9	4	37.4062	38.8845	38.8625	1.3073	-1.4783
3	9	4	67.8461	70.6708	-70.6261	-2.5133	-2.8247
-6	10	4	30.6984	29.1920	29.1485	1.5925	1.5064
-4	10	4	34.6391	33.8115	-33.7305	-2.3382	0.8277
-2	10	4	104.8307	96.7122	96.6586	3.2203	8.1185
0	10	4	39.5112	40.6831	-40.5909	-2.7373	-1.1719
2	10	4	56.6098	58.1244	58.0747	2.4052	-1.5147
-7	11	4	18.6216	18.1512	-18.0351	-2.0502	0.4704
-5	11	4	41.6871	40.1981	40.1430	2.1051	1.4889
-3	11	4	3.9914	4.4237	-4.3431	-0.8404	-0.4322
-1	11	4	13.3962	11.2601	11.2554	0.3269	2.1361
1	11	4	20.8267	20.5629	20.5265	1.2229	0.2638
-6	12	4	7.7046	5.2549	5.1411	1.0879	2.4497
-4	12	4	4.8259	4.5695	-4.2460	-1.6886	0.2564
-2	12	4	13.9630	13.2239	13.0303	2.2545	0.7391
0	12	4	5.0345	4.6776	4.1865	-2.0864	0.3569
2	12	4	13.7990	14.4429	14.3145	1.9217	-0.6438
-3	13	4	29.7578	27.5508	-27.5268	-1.1504	2.2070
-1	13	4	15.2861	15.0895	15.0895	0.0224	0.1966
-10	0	5	66.4578	66.9925	66.9706	1.7127	-0.5347
-8	0	5	29.5296	28.4852	28.4337	-1.7122	1.0443
-6	0	5	101.7493	102.4290	102.3767	3.2731	-0.6797
-4	0	5	88.9965	78.5928	78.5547	-2.4479	10.4037
-2	0	5	63.5418	59.8072	59.7347	2.9440	3.7346
0	0	5	36.8865	35.9300	35.9045	-1.3523	0.9565
2	0	5	55.2561	56.4685	56.4610	0.9217	-1.2124
4	0	5	9.6387	10.4172	-10.4000	0.5979	-0.7785
-9	1	5	18.3487	18.6055	18.4981	1.9959	-0.2568
-7	1	5	7.8302	7.4810	7.4170	-0.9770	0.3491
-5	1	5	60.1156	57.9767	57.9760	0.2948	2.1389
-3	1	5	21.7250	18.9736	-18.9330	1.2399	2.7514
-1	1	5	30.4823	26.4251	26.3508	-1.9799	4.0573
1	1	5	65.8427	66.3175	66.2531	2.9221	-0.4748
3	1	5	28.5618	29.9724	-29.8532	-2.6703	-1.4106
-8	2	5	76.3996	77.2727	-77.2237	-2.7507	-0.8731
-6	2	5	3.4119	2.8594	-0.4247	2.8277	0.5525
-4	2	5	103.3961	96.7663	-96.7005	-3.5692	6.6297
-2	2	5	22.3532	23.6410	23.5094	2.4911	-1.2878
0	2	5	71.2222	69.5347	-69.5080	-1.9272	1.6875
2	2	5	10.6039	11.3965	-11.3947	0.2043	-0.7926

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
4	2	5	7.4823	6.9622	6.9333	0.6337	0.5201
-9	3	5	26.4864	27.5611	27.4959	1.8936	-1.0747
-7	3	5	48.1983	49.2067	-49.1793	-1.6415	-1.0084
-5	3	5	92.3713	88.1169	-88.1150	-0.5806	4.2544
-3	3	5	23.1396	22.2827	22.2474	1.2543	0.8568
-1	3	5	130.5658	127.0862	-127.0482	-3.1095	3.4796
1	3	5	21.6830	22.1372	21.9468	2.8968	-0.4542
3	3	5	78.5295	79.3801	-79.3139	-3.2398	-0.8506
-8	4	5	62.5602	62.9836	-62.9221	-2.7843	-0.4234
-6	4	5	66.6125	65.1138	65.0221	3.4541	1.4987
-4	4	5	124.3224	115.0079	-114.9491	-3.6786	9.3145
-2	4	5	100.2326	95.9960	95.9525	2.8908	4.2366
C	4	5	74.6666	75.2846	-75.2657	-1.6869	-0.6180
2	4	5	27.2174	26.7198	-26.7197	0.0442	0.4976
4	4	5	49.2692	50.7641	50.7509	1.1578	-1.4949
-9	5	5	76.4959	77.4678	77.4252	2.5702	-0.9720
-7	5	5	6.0589	3.1724	3.0354	-0.9220	2.8865
-5	5	5	6.3003	6.1705	-6.1689	0.1396	0.1298
-3	5	5	108.9013	96.3299	96.3095	1.9812	12.5713
-1	5	5	56.5085	55.3848	-55.3298	-2.4680	1.1237
1	5	5	116.5542	118.1626	118.1107	3.5009	-1.6084
3	5	5	25.0203	25.3944	-25.2507	-2.6979	-0.3741
-8	6	5	14.4797	13.9628	-13.8101	-2.0593	0.5169
-6	6	5	112.3403	111.4330	111.3795	3.4523	0.9074
-4	6	5	5.3590	3.3836	-1.8997	-2.7999	1.9754
-2	6	5	90.6228	86.6799	86.6309	2.9123	3.9430
0	6	5	10.4734	7.7843	7.6811	-1.2633	2.6891
2	6	5	18.8940	17.5663	17.5598	0.4779	1.3277
4	6	5	31.2764	31.3749	31.3593	0.9915	-0.0985
-7	7	5	9.8333	10.3623	-10.3050	-1.1073	-0.5290
-5	7	5	35.4147	33.7121	33.7121	0.0360	1.7026
-3	7	5	26.7114	23.9185	-23.8988	0.9691	2.7929
-1	7	5	10.6932	11.6491	-11.4631	-2.0734	-0.9559
1	7	5	43.9573	44.7156	44.6443	2.5238	-0.7583
3	7	5	49.4509	50.0466	-49.9787	-2.6059	-0.5956
-8	8	5	62.1428	63.3713	-63.3309	-2.2627	-1.2285
-6	8	5	32.4137	29.0766	-29.0102	1.9631	3.3371
-4	8	5	46.7132	45.2656	-45.1741	-2.8770	1.4476
-2	8	5	34.5024	32.1769	-32.1251	1.8246	2.3255
0	8	5	40.8858	39.5716	-39.5320	-1.7691	1.3142
2	8	5	6.5921	4.1383	4.1259	0.3211	2.4537
-7	9	5	19.7875	19.1349	-19.1016	-1.1294	0.6526
-5	9	5	6.8797	6.5657	-6.5646	-0.1196	0.3141
-3	9	5	57.4438	51.6961	-51.6929	0.5784	5.7477
-1	9	5	4.7332	4.8420	-4.4846	-1.8258	-0.1088
1	9	5	7.7373	5.3723	-4.9873	1.9970	2.3650
-6	10	5	32.6103	32.9701	32.8732	2.5261	-0.3597
-4	10	5	6.1289	7.4724	-7.1145	-2.2851	-1.3435
-2	10	5	54.3942	52.7261	52.6752	2.3150	1.6681
0	10	5	28.7918	27.9127	-27.8847	-1.2500	0.8792
2	10	5	14.8235	13.2719	13.2620	0.5110	1.5516
-5	11	5	3.7456	1.6156	-1.6003	0.2216	2.1300
-3	11	5	60.9894	56.2628	56.2426	1.5075	4.7265
-1	11	5	14.5021	15.4465	-15.3519	-1.7071	-0.9444
1	11	5	58.4891	57.9107	57.8502	2.6475	0.5784

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-4	12	5	51.7232	47.5400	-47.4704	-2.5704	4.1832
-2	12	5	63.1974	61.2217	61.1800	2.2600	1.9757
-8	0	6	75.8171	74.7173	-74.6462	-3.2590	1.0998
-6	0	6	42.9516	41.4484	41.3675	2.5883	1.5032
-4	0	6	45.7151	42.2238	-42.1873	-1.7559	3.4913
-2	0	6	51.2017	48.5700	-48.5698	-0.1357	2.6318
0	0	6	3.9914	2.9411	-2.7707	0.9867	1.0503
2	0	6	80.2972	76.3364	-76.2958	-2.4880	3.9608
-9	1	6	9.1515	9.0956	9.0952	-0.0783	0.0560
-7	1	6	41.2370	40.4817	40.4557	1.4517	0.7553
-5	1	6	95.0275	90.8225	-90.7802	-2.7720	4.2051
-3	1	6	120.8180	118.4134	118.3654	3.3697	2.4047
-1	1	6	78.3845	79.4929	-79.4200	-3.4029	-1.1084
1	1	6	35.7230	34.1230	34.0323	2.4871	1.6000
3	1	6	11.3959	9.8158	-9.6929	-1.5486	1.5801
-8	2	6	41.7186	42.3908	-42.2996	-2.7781	-0.6722
-6	2	6	69.5740	67.6121	67.5620	2.6026	1.9619
-4	2	6	5.3640	6.6095	-6.4515	-1.4367	-1.2455
-2	2	6	23.9158	23.0832	23.0784	0.4699	0.8326
0	2	6	49.0498	46.5199	46.5063	1.1275	2.5299
2	2	6	5.0160	5.2783	-5.0164	-1.6419	-0.2623
-9	3	6	7.3524	6.2792	-6.2791	-0.0217	1.0733
-7	3	6	0.0000	1.1597	0.3098	1.1176	-1.1597
-5	3	6	11.6007	9.7402	-9.5462	-1.9344	1.8605
-3	3	6	5.0901	3.1471	1.4357	2.8005	1.9430
-1	3	6	11.2248	8.9544	-8.5613	-2.6239	2.2704
1	3	6	45.0296	43.8578	43.7769	2.6628	1.1718
3	3	6	36.4478	35.2769	-35.2462	-1.4731	1.1709
-8	4	6	21.2662	22.2106	-22.0851	-2.3581	-0.9444
-6	4	6	29.1953	30.0375	29.9580	2.1839	-0.8422
-4	4	6	40.5713	38.5637	-38.5330	-1.5374	2.0076
-2	4	6	5.6001	4.3392	4.3071	0.5269	1.2609
0	4	6	12.7043	9.6127	-9.5979	0.5319	3.0916
2	4	6	0.0000	2.0929	1.6038	-1.3446	-2.0929
-7	5	6	15.1811	14.3986	-14.3734	0.8518	0.7826
-5	5	6	4.2509	2.1065	0.8005	-1.9485	2.1444
-3	5	6	6.9772	6.0128	-5.5452	2.3248	0.9644
-1	5	6	20.4859	21.9809	-21.8003	-2.8115	-1.4949
1	5	6	22.3943	21.8503	21.7447	2.1452	0.5440
-8	6	6	31.0822	31.2252	-31.1235	-2.5190	-0.1431
-6	6	6	18.1347	18.5259	18.4045	2.1175	-0.3912
-4	6	6	32.6984	31.2533	-31.2137	-1.5724	1.4451
-2	6	6	20.5554	19.2733	-19.2725	0.1728	1.2822
0	6	6	29.1919	26.7771	-26.7725	0.4973	2.4148
2	6	6	26.3073	25.1715	-25.1099	-1.7603	1.1358
-7	7	6	27.4026	27.2250	27.1951	1.2761	0.1776
-5	7	6	61.9121	59.1597	-59.1151	-2.2963	2.7525
-3	7	6	91.7535	90.0545	90.0041	3.0098	1.6990
-1	7	6	56.0250	56.2816	-56.2088	-2.8623	-0.2566
1	7	6	36.9155	34.8423	34.7643	2.3309	2.0732
-6	8	6	71.9574	69.2310	69.1860	2.4959	2.7265
-4	8	6	14.8954	13.9449	13.8972	-1.1519	0.9505
-2	8	6	25.0129	24.5581	24.5559	0.3289	0.4549
0	8	6	67.1151	63.5219	63.5070	1.3764	3.5932
-7	9	6	40.7385	39.8793	39.8567	1.3445	0.8592

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-5	9	6	76.9873	73.3069	-73.2702	-2.3192	3.6805
-3	9	6	90.2116	86.6399	86.5872	3.0235	3.5717
-1	9	6	46.7381	47.2511	-47.1745	-2.6895	-0.5130
-6	10	6	33.5919	33.0171	32.9566	1.9987	0.5748
-4	10	6	48.7275	46.6300	-46.6091	-1.3950	2.0975
-2	10	6	30.5719	32.0245	-32.0245	0.0152	-1.4526
-3	11	6	0.0000	2.4472	1.4627	1.9619	-2.4472
-8	0	7	44.9018	46.1689	-46.1389	-1.6646	-1.2671
-6	0	7	42.9299	39.9557	-39.9557	-0.0578	2.9742
-4	0	7	65.9912	65.2517	-65.2516	0.0809	0.7395
-2	0	7	24.1184	25.6269	-25.5577	-1.8821	-1.5085
0	0	7	25.3614	22.5128	-22.4470	1.7210	2.8486
-7	1	7	10.2089	8.8557	-8.5926	2.1425	1.3533
-5	1	7	26.7203	26.6449	-26.4999	-2.7752	0.0754
-3	1	7	27.4733	28.1121	28.0206	2.2669	-0.6387
-1	1	7	55.9446	55.9035	-55.8702	-1.9291	0.0411
1	1	7	19.9707	16.6080	16.5949	0.6599	3.3627
-8	2	7	16.9958	16.7918	16.7639	-0.9682	0.2039
-6	2	7	45.6941	43.1191	43.1147	0.6150	2.5751
-4	2	7	39.6975	39.6006	39.5833	1.1704	0.0969
-2	2	7	0.0000	1.5688	-0.0276	-1.5685	-1.5688
0	2	7	64.0889	61.9219	61.8635	2.6875	2.1670
-7	3	7	90.4164	88.3513	88.2905	3.2791	2.0650
-5	3	7	29.5037	29.3548	-29.2367	-2.6300	0.1490
-3	3	7	73.5950	75.0206	74.9625	2.9503	-1.4256
-1	3	7	14.7091	13.9672	13.9168	-1.1866	0.7418
1	3	7	18.1618	16.7133	16.6980	0.7163	1.4485
-8	4	7	27.5696	26.7979	-26.7657	-1.3119	0.7718
-6	4	7	4.3808	2.8543	-2.8505	0.1483	1.5264
-4	4	7	30.6438	29.9684	29.9430	1.2344	0.6754
-2	4	7	66.3476	68.9903	-68.9535	-2.2527	-2.6427
0	4	7	75.6963	73.5208	73.4677	2.7915	2.1755
-7	5	7	46.4833	46.7324	46.6634	2.5338	-0.2491
-5	5	7	104.4857	100.2894	-100.2316	-3.4041	4.1964
-3	5	7	15.5086	16.2676	16.1272	2.1329	-0.7590
-1	5	7	48.0507	48.5386	-48.5036	-1.8419	-0.4878
-6	6	7	41.1315	38.7465	-38.7461	-0.1746	2.3850
-4	6	7	19.4439	18.6053	-18.5969	0.5579	0.8386
-2	6	7	56.8645	59.0702	-59.0297	-2.1873	-2.2057
0	6	7	21.3706	20.2147	20.1081	2.0737	1.1559
-7	7	7	20.1200	19.4517	19.3207	2.2534	0.6683
-5	7	7	11.8613	12.7903	-12.5801	-2.3094	-0.9290
-3	7	7	51.2452	52.1025	52.0510	2.3175	-0.8573
-1	7	7	20.6131	19.9038	-19.8509	-1.4500	0.7093
-6	8	7	58.9828	56.3270	56.3209	0.8278	2.6559
-4	8	7	31.3641	32.1043	32.0917	0.9002	-0.7403
-2	8	7	44.9467	45.6737	45.6661	-0.8300	-0.7270
-3	9	7	38.0318	38.5965	38.5344	2.1879	-0.5646
-6	0	8	40.6053	40.6171	-40.5598	-2.1563	-0.0118
-4	0	8	65.9713	68.3932	68.3344	2.8354	-2.4220
-2	0	8	17.6796	18.8820	-18.6950	-2.6511	-1.2024
-7	1	8	64.0529	62.1240	62.0781	2.3880	1.9289
-5	1	8	22.2787	23.1609	-23.1110	-1.5192	-0.8823
-3	1	8	18.2465	19.4939	-19.4910	0.3370	-1.2474
-1	1	8	45.5840	46.7883	46.7804	0.8623	-1.2043

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-6	2	8	39.9194	40.2519	-40.2114	-1.8058	-0.3325
-4	2	8	30.2556	32.0058	31.9162	2.3921	-1.7501
-2	2	8	46.1747	48.1531	-48.0816	-2.6230	-1.9785
-5	3	8	12.4448	11.9959	-11.9029	-1.4909	0.4489
-3	3	8	24.5045	26.2962	26.2875	0.6779	-1.7917
-6	4	8	11.2115	11.8112	-11.7357	-1.3328	-0.5997
-4	4	8	14.3066	16.6421	16.5264	1.9590	-2.3354
-2	4	8	25.5014	26.7087	-26.6135	-2.2530	-1.2073
-5	5	8	25.3257	25.7466	-25.7036	-1.4863	-0.4209
-3	5	8	18.9002	19.6851	19.6708	0.7515	-0.7849
10	0	0	72.1331	68.6015	68.5767	1.8448	3.5316
11	1	0	43.7000	42.2380	42.1943	1.9206	1.4621
10	2	0	3.8464	3.7660	3.6266	1.0153	0.0804
11	3	0	6.6721	6.9527	-6.8009	1.4451	-0.2806
10	4	0	19.1440	18.4062	-18.3905	0.7593	0.7378
9	5	0	6.7559	5.9701	5.6076	-2.0485	0.7859
11	5	0	35.6493	34.5681	34.5170	1.8797	1.0812
10	6	0	26.2443	24.1258	24.0947	1.2252	2.1185
9	7	0	57.4519	55.5869	-55.5268	-2.5835	1.8650
8	8	0	57.0059	55.2745	-55.2690	-0.7804	1.7314
10	8	0	21.5406	21.1588	21.1309	1.0869	0.3817
9	9	0	61.2947	59.5501	-59.4943	-2.5784	1.7446
8	10	0	10.2211	9.7176	9.7172	-0.0896	0.5035
10	10	0	25.8221	25.2970	25.2683	1.2051	0.5251
7	11	0	43.2956	41.5784	41.4967	2.6061	1.7172
9	11	0	0.0000	2.2323	1.4984	-1.6547	-2.2323
6	12	0	17.6975	17.8284	-17.8110	-0.7890	-0.1309
8	12	0	29.9171	30.0198	30.0194	0.1666	-0.1027
7	13	0	13.6880	14.3632	-14.2789	1.5537	-0.6753
6	14	0	26.1906	25.4803	-25.4602	-1.0119	0.7103
8	14	0	9.2370	8.9284	-8.9246	-0.2630	0.3086
3	15	0	12.4047	12.7839	12.7128	1.3464	-0.3792
5	15	0	15.1155	14.9787	-14.8680	-1.8177	0.1368
7	15	0	26.4565	25.5530	25.4800	1.9293	0.9036
0	16	0	109.0688	110.0955	110.0552	2.9782	-1.0267
2	16	0	18.4252	18.1802	-18.0789	-1.9170	0.2450
4	16	0	51.5252	51.6180	51.5847	1.8532	-0.0928
6	16	0	22.2794	22.6052	22.6037	-0.2571	-0.3258
1	17	0	3.0072	3.9040	-3.8924	-0.2998	-0.8968
3	17	0	53.9834	55.1138	55.0876	1.7006	-1.1304
5	17	0	29.8554	29.9314	-29.8822	-1.7159	-0.0761
0	18	0	25.9455	24.3658	24.2813	2.0264	1.5798
2	18	0	51.4022	53.0756	-53.0347	-2.0831	-1.6733
4	18	0	5.9399	4.8541	4.7127	1.1631	1.0858
1	19	0	28.7136	29.0417	-29.0333	-0.7008	-0.3281
3	19	0	6.0378	4.7072	4.6549	0.6994	1.3306
-12	0	1	36.1782	37.2534	37.2515	0.3671	-1.0752
-10	0	1	16.7294	14.9771	14.9594	-0.7284	1.7523
10	0	1	13.2300	12.3822	-12.2406	1.8673	0.8478
-11	1	1	19.9088	18.3364	18.1977	2.2509	1.5724
9	1	1	14.8921	15.1073	-15.0545	-1.2617	-0.2152
11	1	1	8.9620	9.2342	9.2314	0.2257	-0.2722
-12	2	1	13.7105	12.9380	-12.9351	-0.2723	0.7725
-10	2	1	30.2677	29.6491	-29.6295	-1.0778	0.6186
10	2	1	38.4882	35.0229	34.9436	2.3552	3.4653

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-11	3	1	28.2366	26.2081	26.1068	2.3018	2.0285
9	3	1	9.3396	8.8670	-8.8151	-0.9585	0.4726
-10	4	1	4.5831	4.7064	-4.6384	-0.7969	-0.1233
10	4	1	50.8295	47.4589	47.3919	2.5203	3.3706
-11	5	1	52.8290	51.4268	51.3572	2.6735	1.4022
9	5	1	7.5022	7.5438	-7.4709	-1.0464	-0.0416
-10	6	1	22.0060	20.3928	20.3849	-0.5682	1.6132
8	6	1	49.8489	47.3908	-47.3358	-2.2822	2.4581
10	6	1	16.0019	15.0306	14.8888	2.0598	0.9713
-11	7	1	20.2122	18.4968	18.3908	1.9774	1.7154
-9	7	1	11.2431	11.8683	-11.6945	-2.0236	-0.6251
9	7	1	12.5070	11.9701	-11.9227	-1.0638	0.5369
-10	8	1	35.8620	35.5163	-35.4991	-1.1039	0.3458
8	8	1	28.6383	27.5424	27.5050	-1.4338	1.0959
10	8	1	17.6724	15.8888	15.7804	1.8530	1.7836
-9	9	1	14.0839	13.4807	-13.3569	-1.8227	0.6032
7	9	1	18.5233	17.5577	17.4536	1.9086	0.9656
9	9	1	7.8847	8.4466	-8.3911	-0.9669	-0.5619
-10	10	1	3.4268	3.9149	-3.8589	-0.6597	-0.4881
-8	10	1	34.7325	34.0814	34.0360	1.7596	0.6511
8	10	1	27.5680	27.2809	-27.2280	-1.6988	0.2871
-9	11	1	28.9369	28.3227	-28.2663	-1.7859	0.6143
-7	11	1	39.5423	39.5356	39.4987	1.7086	0.0067
7	11	1	16.2494	15.3949	15.3018	1.6902	0.8545
9	11	1	11.2381	10.9698	-10.9316	-0.9139	0.2684
-8	12	1	26.1440	25.4556	25.4004	1.6750	0.6883
6	12	1	50.2057	50.4737	50.4532	1.4393	-0.2680
8	12	1	52.4451	51.3671	-51.3283	-1.9953	1.0781
-9	13	1	43.3359	44.3640	-44.3141	-2.1032	-1.0280
-7	13	1	38.6097	38.8969	38.8682	1.4939	-0.2872
5	13	1	59.8756	61.5876	-61.5354	-2.5349	-1.7120
7	13	1	25.1597	25.3282	25.2727	1.6763	-0.1686
-8	14	1	4.7182	3.2188	2.9825	1.2106	1.4994
-6	14	1	60.6101	60.0393	-59.9910	-2.4068	0.5707
4	14	1	7.5908	7.6009	-7.5955	-0.2880	-0.0101
6	14	1	44.4628	45.2013	45.1824	1.3055	-0.7385
-7	15	1	12.0634	11.0792	11.0292	1.0512	0.9842
-5	15	1	5.7627	5.1600	-5.1438	-0.4085	0.6028
-3	15	1	10.0299	9.2440	-9.2298	-0.5127	0.7859
3	15	1	41.8781	43.2458	43.1878	2.2392	-1.3677
5	15	1	26.4710	25.2480	-25.1747	-1.9223	1.2231
7	15	1	25.0446	23.6957	23.6529	1.4229	1.3489
-6	16	1	3.0398	3.6057	3.3210	-1.4043	-0.5659
-4	16	1	15.6193	15.0081	14.8872	1.9012	0.6112
-2	16	1	18.6403	20.7472	20.6893	-1.5488	-2.1069
0	16	1	1.0677	1.3426	0.2448	1.3201	-0.2749
2	16	1	15.3132	16.2087	-16.1945	-0.6785	-0.8956
4	16	1	8.5467	8.1114	8.1113	-0.0316	0.4354
6	16	1	16.0092	18.2691	-18.2613	0.5352	-2.2599
-5	17	1	6.4063	6.4810	6.4803	-0.0974	-0.0747
-3	17	1	1.8509	1.0356	-0.9895	-0.3055	0.8153
-1	17	1	1.7250	1.4493	-1.0591	0.9893	0.2758
1	17	1	0.0000	1.3735	-0.2547	-1.3496	-1.3735
3	17	1	0.0000	1.8386	1.0325	1.5213	-1.8386
5	17	1	13.1643	11.7241	-11.6290	-1.4900	1.4402

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-4	18	1	6.7285	9.5909	-9.4836	1.4303	-2.8624
-2	18	1	0.0000	1.7953	-1.0762	-1.4370	-1.7953
0	18	1	0.0000	2.0607	-1.7710	1.0536	-2.0607
2	18	1	15.6124	17.1624	-17.1512	-0.6176	-1.5500
4	18	1	12.1064	13.0235	13.0235	-0.0032	-0.9171
-3	19	1	15.9741	15.2597	-15.2522	-0.4786	0.7144
-1	19	1	5.4178	4.4748	4.3801	0.9159	0.9430
1	19	1	13.3582	14.4298	-14.3553	-1.4644	-1.0716
-12	0	2	7.8614	8.7101	8.5896	1.4436	-0.8486
-10	0	2	60.6481	58.7275	-58.6523	-2.9717	1.9206
0	0	2	199.5094	198.7465	-198.7433	-1.1341	0.7629
8	0	2	79.1952	76.5372	-76.4717	-3.1660	2.6579
10	0	2	3.0631	2.9346	2.5087	1.5227	0.1285
-11	1	2	29.5119	28.3049	28.2622	1.5553	1.2070
9	1	2	22.9279	21.3308	21.3055	1.0372	1.5971
-12	2	2	29.9742	28.5054	28.4549	1.6964	1.4688
-10	2	2	28.8842	28.6775	-28.5778	-2.3893	0.2067
8	2	2	25.3853	24.7589	-24.6413	-2.4106	0.6264
10	2	2	37.4710	35.5374	35.4800	2.0181	1.9336
-11	3	2	20.4644	18.6854	18.6361	1.3569	1.7790
9	3	2	21.0588	19.4743	19.4491	0.9921	1.5845
-12	4	2	28.3650	27.0724	27.0291	1.5300	1.2926
-10	4	2	29.9416	29.6634	-29.5791	-2.2352	0.2782
8	4	2	29.9440	29.3945	-29.2997	-2.3594	0.5494
10	4	2	29.9961	28.4917	28.4329	1.8285	1.5045
-11	5	2	21.4526	21.6254	-21.6093	0.8334	-0.1728
9	5	2	27.4488	27.4620	-27.4604	0.2951	-0.0131
-10	6	2	38.3351	36.4923	-36.4115	-2.4259	1.8428
8	6	2	49.8710	48.3817	-48.3096	-2.6409	1.4893
-11	7	2	29.9223	29.9759	29.9407	1.4522	-0.0537
-9	7	2	14.1214	13.3584	13.3511	-0.4409	0.7630
7	7	2	13.4634	12.1801	12.1799	0.0718	1.2832
9	7	2	29.7845	29.6273	29.6086	1.0522	0.1572
-10	8	2	20.2607	19.9123	-19.7958	-2.1510	0.3484
8	8	2	17.5614	16.5606	-16.4271	-2.0981	1.0009
-11	9	2	39.9845	39.7808	39.7509	1.5416	0.2038
-9	9	2	7.2130	6.8591	-6.8409	-0.4993	0.3539
7	9	2	5.0354	4.5036	4.5034	0.0446	0.5317
9	9	2	36.5490	36.2663	36.2460	1.2150	0.2826
-10	10	2	46.1874	45.3357	-45.2802	-2.2427	0.8517
-8	10	2	21.8515	22.5104	22.3734	2.4796	-0.6589
6	10	2	26.2631	26.7258	26.6222	2.3509	-0.4627
8	10	2	53.5337	52.2510	-52.1979	-2.3547	1.2828
-9	11	2	27.4306	26.6788	-26.6721	-0.5957	0.7518
7	11	2	20.2057	19.9167	-19.9157	-0.2005	0.2890
-10	12	2	21.9188	21.3481	-21.2820	-1.6788	0.5707
-8	12	2	0.0000	2.1450	-1.0600	1.8647	-2.1450
6	12	2	9.2419	9.3738	-9.2121	1.7335	-0.1319
8	12	2	23.4541	23.3807	-23.3089	-1.8307	0.0734
-9	13	2	27.0664	28.6902	28.6901	0.0591	-1.6237
-7	13	2	14.7658	14.7775	14.7746	-0.2931	-0.0117
5	13	2	4.6157	3.7445	-3.6623	-0.7799	0.8712
7	13	2	34.0695	35.5443	35.5399	0.5551	-1.4748
-8	14	2	29.1259	28.9317	28.8621	2.0058	0.1942
-6	14	2	12.1531	12.8897	12.7999	-1.5190	-0.7367

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
4	14	2	30.8319	33.1134	33.0935	-1.1485	-2.2815
6	14	2	30.9925	30.6195	30.5534	2.0108	0.3730
-7	15	2	9.9601	10.0845	-10.0730	-0.4809	-0.1244
-5	15	2	21.9161	21.7673	21.7273	1.3185	0.1488
-3	15	2	20.4811	20.5109	-20.4120	-2.0114	-0.0297
1	15	2	16.8534	17.2835	-17.1474	-2.1650	-0.4301
3	15	2	23.5055	24.3420	24.2871	1.6332	-0.8365
5	15	2	9.8813	11.0116	-10.9807	-0.8248	-1.1303
-6	16	2	65.3494	64.5165	-64.4749	-2.3163	0.8329
-4	16	2	16.0551	16.3080	16.2551	1.3123	-0.2529
-2	16	2	61.5932	60.6220	-60.6119	-1.1072	0.9712
0	16	2	47.7385	50.8493	-50.8444	-0.7049	-3.1108
2	16	2	5.3664	4.0687	3.9616	0.9274	1.2977
4	16	2	66.1919	69.2086	-69.1749	-2.1594	-3.0167
-5	17	2	13.8131	12.5840	12.5348	1.1113	1.2291
-3	17	2	76.1388	75.1854	-75.1490	-2.3399	0.9534
-1	17	2	45.9570	41.0186	40.9614	2.1649	4.9384
1	17	2	56.2490	61.3225	-61.2744	-2.4295	-5.0735
3	17	2	5.9678	4.1568	-3.9719	1.2258	1.8110
-4	18	2	37.7595	36.4061	36.3762	1.4737	1.3535
-2	18	2	4.7090	3.1473	-3.1063	-0.5067	1.5617
0	18	2	2.9932	1.7733	1.7652	-0.1691	1.2199
2	18	2	30.2342	33.5566	33.5353	1.1954	-3.3224
-3	19	2	10.3423	8.2541	-8.1666	-1.1981	2.0882
-1	19	2	51.0380	45.7163	45.6716	2.0208	5.3217
1	19	2	9.7783	8.0983	-7.9929	-1.3021	1.6800
-12	0	3	12.3300	12.4484	-12.3319	1.6992	-0.1185
8	0	3	21.5317	22.6827	-22.6360	-1.4541	-1.1509
-11	1	3	15.7650	16.1724	-16.1535	-0.7808	-0.4073
9	1	3	17.0012	15.5473	15.4287	1.9167	1.4538
-12	2	3	43.6349	41.9598	41.8868	2.4738	1.6751
8	2	3	20.6221	20.0377	-19.9954	-1.3007	0.5844
-11	3	3	15.7791	16.3043	16.3022	-0.2599	-0.5251
7	3	3	24.8171	24.2918	-24.2057	-2.0432	0.5253
9	3	3	29.7298	27.6190	27.5338	2.1670	2.1108
-12	4	3	41.6021	40.3879	40.3081	2.5372	1.2142
-10	4	3	58.4985	57.3459	-57.2803	-2.7409	1.1527
8	4	3	0.0000	1.0894	0.0974	-1.0850	-1.0894
-11	5	3	13.2539	13.4216	-13.4002	-0.7567	-0.1677
7	5	3	54.5955	53.3046	-53.2599	-2.1833	1.2908
9	5	3	25.5913	24.7825	24.6905	2.1333	0.8088
-12	6	3	13.2393	12.3071	12.1506	1.9561	0.9322
-10	6	3	72.5049	71.8427	-71.7922	-2.6931	0.6623
8	6	3	4.3593	4.4477	-4.3023	-1.1282	-0.0884
-11	7	3	7.0590	5.8155	-5.7914	-0.5285	1.2435
7	7	3	14.4023	14.1935	-14.1084	-1.5516	0.2089
-10	8	3	19.3980	19.8474	19.7921	-1.4806	-0.4493
6	8	3	14.2347	14.2571	14.1122	2.0274	-0.0224
8	8	3	28.8934	28.8894	-28.8614	-1.2714	0.0040
-11	9	3	4.0842	4.3989	4.3823	-0.3814	-0.3147
-9	9	3	18.8230	18.5140	18.4502	1.5355	0.3089
7	9	3	4.0142	1.3062	0.2912	-1.2733	2.7080
-10	10	3	30.3996	29.8550	-29.7902	-1.9660	0.5446
-8	10	3	17.5298	17.2587	-17.2100	1.2957	0.2711
6	10	3	24.3625	23.7088	23.6379	1.8323	0.6537

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
8	10	3	13.6828	12.4780	-12.4299	-1.0949	1.2048
-9	11	3	6.8866	6.6148	6.5179	1.1281	0.2718
5	11	3	3.0678	2.4610	2.2926	0.8948	0.6067
7	11	3	24.9981	24.4707	-24.4200	-1.5748	0.5274
-10	12	3	46.5130	46.3454	-46.2945	-2.1729	0.1676
-8	12	3	33.6550	33.4789	33.4384	1.6481	0.1761
4	12	3	64.9452	67.2223	-67.1728	-2.5794	-2.2771
6	12	3	22.9549	22.4931	22.4263	1.7314	0.4619
-9	13	3	35.5337	36.5810	36.5482	1.5491	-1.0473
-7	13	3	46.3888	46.1735	-46.1246	-2.1233	0.2153
3	13	3	2.8206	0.6126	0.6091	-0.0653	2.2081
5	13	3	46.9290	50.7005	50.6850	1.2548	-3.7716
-8	14	3	61.3393	62.4155	62.3898	1.7937	-1.0762
-6	14	3	16.9565	17.3030	17.2976	-0.4316	-0.3465
2	14	3	57.7103	61.0047	60.9507	2.5650	-3.2944
4	14	3	25.5107	26.7594	-26.6781	-2.0843	-1.2487
6	14	3	15.4432	15.1106	15.0328	1.5318	0.3326
-7	15	3	9.1577	8.5503	-8.3914	-1.6405	0.6075
-5	15	3	25.7296	24.7599	24.6720	2.0845	0.9698
-3	15	3	17.5666	15.4287	-15.2934	-2.0388	2.1379
-1	15	3	39.2664	35.5243	35.4842	1.6873	3.7422
1	15	3	27.2915	29.1825	-29.1664	-0.9687	-1.8910
3	15	3	3.4454	2.5865	2.5861	0.0473	0.8589
5	15	3	10.8330	11.3747	11.3557	0.6576	-0.5417
-6	16	3	15.7978	15.5282	-15.5131	-0.6847	0.2696
-4	16	3	30.3844	30.6027	-30.5995	-0.4386	-0.2183
-2	16	3	22.8002	22.0846	-22.0760	0.6157	0.7156
0	16	3	4.7095	5.8002	-5.6039	-1.4961	-1.0907
2	16	3	3.9258	5.2534	-5.0357	1.4968	-1.3276
4	16	3	8.7010	8.7425	-8.5860	-1.6463	-0.0414
-5	17	3	14.4704	16.9578	-16.9124	1.2402	-2.4874
-3	17	3	14.1045	11.7659	-11.6525	-1.6296	2.3386
-1	17	3	7.3824	7.5142	-7.4346	1.0908	-0.1318
1	17	3	23.3944	25.2163	-25.1995	-0.9204	-1.8219
3	17	3	8.9892	5.0247	5.0220	0.1668	3.9645
-4	18	3	7.1623	8.1671	8.1668	-0.0647	-1.0048
-2	18	3	8.9368	9.7285	-9.7026	0.7096	-0.7918
0	18	3	5.5350	6.3685	6.2777	-1.0717	-0.8336
2	18	3	5.1476	6.6637	6.5108	1.4192	-1.5161
-1	19	3	20.9883	18.5829	18.5342	1.3447	2.4054
-12	0	4	47.7895	46.8943	46.8556	1.9045	0.8953
8	0	4	58.7069	58.2850	58.2708	1.2870	0.4219
-11	1	4	40.9232	41.2496	-41.1799	-2.3976	-0.3265
7	1	4	29.4063	28.4845	-28.3836	-2.3949	0.9218
-12	2	4	15.2929	14.6569	14.5858	1.4413	0.6360
6	2	4	17.2095	16.8319	-16.8317	0.0876	0.3775
8	2	4	3.3568	2.2676	-2.2257	0.4336	1.0893
-11	3	4	29.7155	29.7657	-29.6875	-2.1556	-0.0502
7	3	4	58.7493	58.5788	-58.5191	-2.6425	0.1706
-12	4	4	10.0721	10.1676	-10.1075	1.1037	-0.0954
-10	4	4	9.6523	9.2094	9.1937	-0.5388	0.4428
6	4	4	22.1643	22.2263	22.2186	0.5855	-0.0620
8	4	4	20.3989	19.7283	-19.7271	0.2129	0.6706
-11	5	4	0.0000	3.0402	2.4740	-1.7670	-3.0402
7	5	4	10.0349	9.3474	-9.1493	-1.9141	0.6875

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-12	6	4	16.8151	16.6489	16.5939	1.3528	0.1662
-10	6	4	5.2125	4.3915	4.3566	-0.5529	0.8210
6	6	4	42.5858	43.0642	43.0583	0.7129	-0.4785
8	6	4	18.7779	18.3145	18.3002	0.7225	0.4634
-11	7	4	36.8197	36.1619	-36.0975	-2.1578	0.6578
5	7	4	44.9182	45.5365	45.4682	2.4928	-0.6183
7	7	4	34.9867	33.9978	-33.9210	-2.2846	0.9889
-10	8	4	29.1207	28.9074	-28.8912	-0.9687	0.2133
6	8	4	33.9055	35.0648	-35.0637	-0.2751	-1.1593
-11	9	4	46.2913	47.0672	-47.0179	-2.1518	-0.7759
-9	9	4	57.1931	57.6172	57.5526	2.7248	-0.4241
5	9	4	29.5606	30.0131	29.9252	2.2950	-0.4524
7	9	4	44.5332	44.6982	-44.6381	-2.3173	-0.1650
-10	10	4	5.9306	5.4665	-5.4340	-0.5958	0.4641
-8	10	4	7.3808	6.0213	6.0177	-0.2090	1.3595
4	10	4	4.2241	3.2962	-3.1289	-1.0369	0.9279
6	10	4	5.8187	4.6325	4.6220	0.3109	1.1862
-9	11	4	25.4473	25.2826	25.1850	2.2195	0.1647
-7	11	4	18.4563	18.1512	-18.0351	-2.0502	0.3050
3	11	4	9.9008	10.6460	10.5652	-1.3092	-0.7452
5	11	4	35.6461	36.5949	36.5269	2.2289	-0.9488
-10	12	4	7.2413	8.4833	8.4754	-0.3651	-1.2419
-8	12	4	3.8651	3.3898	-3.3809	-0.2455	0.4753
2	12	4	14.1073	14.4429	14.3145	1.9217	-0.3355
4	12	4	13.1761	13.3014	-13.2547	-1.1133	-0.1253
6	12	4	26.3687	27.5660	27.5596	0.5929	-1.1973
-9	13	4	16.2849	17.8098	-17.7511	1.4443	-1.5249
-7	13	4	0.0000	1.8363	-0.2331	-1.8214	-1.8363
-5	13	4	8.2532	6.9873	6.8563	1.3468	1.2659
1	13	4	25.4886	24.9565	-24.9538	0.3619	0.5321
3	13	4	3.5340	2.3125	-1.8468	-1.3918	1.2215
5	13	4	0.0000	2.6348	-2.2855	1.3111	-2.6348
-8	14	4	7.5257	8.1046	-8.0966	-0.3590	-0.5789
-6	14	4	5.8609	5.9927	-5.9406	0.7885	-0.1318
-4	14	4	36.3797	34.6778	-34.6276	-1.8659	1.7019
-2	14	4	6.9160	7.4163	-7.2077	1.7466	-0.5003
0	14	4	31.1148	29.9445	-29.8583	-2.2705	1.1703
2	14	4	12.1147	13.9701	-13.9062	1.3350	-1.8555
4	14	4	34.2796	37.8062	-37.7823	-1.3431	-3.5266
-7	15	4	21.3993	20.9515	-20.8714	-1.8299	0.4478
-5	15	4	26.9150	25.9769	25.9289	1.5785	0.9381
-3	15	4	14.7938	12.5200	-12.4902	-0.8626	2.2739
-1	15	4	11.7273	10.5651	-10.5650	-0.0431	1.1622
1	15	4	13.7490	14.2189	14.1933	0.8523	-0.4699
3	15	4	17.1741	17.1252	-17.0669	-1.4127	0.0489
-6	16	4	29.3903	29.5826	29.5544	1.2933	-0.1923
-4	16	4	18.5813	16.8479	-16.7684	-1.6349	1.7335
-2	16	4	84.3622	78.8321	78.7909	2.5497	5.5300
0	16	4	17.6548	17.4146	-17.3160	-1.8509	0.2402
2	16	4	48.3145	51.3747	51.3406	1.8706	-3.0601
-5	17	4	40.1189	39.4770	39.4409	1.6877	0.6419
-3	17	4	0.0000	3.7022	3.6545	-0.5923	-3.7022
-1	17	4	13.5405	15.5828	-15.5827	-0.0336	-2.0423
1	17	4	40.8401	42.6653	42.6474	1.2346	-1.8252
-4	18	4	45.3904	45.9194	-45.8870	-1.7269	-0.5290

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-2	18	4	29.2649	27.0220	26.9600	1.8302	2.2429
0	18	4	46.5652	48.0659	-48.0266	-1.9433	-1.5007
-12	0	5	33.4158	34.6368	34.6367	0.0532	-1.2209
6	0	5	28.5184	28.6990	28.6821	-0.9860	-0.1806
-11	1	5	8.3701	9.3863	9.1945	-1.8876	-1.0162
5	1	5	46.3176	45.1227	45.0612	2.3560	1.1949
7	1	5	16.5786	15.5402	-15.4774	-1.3953	1.0385
-12	2	5	22.7323	23.5821	-23.5752	-0.5695	-0.8498
-10	2	5	12.4191	11.9450	-11.8948	1.0936	0.4740
6	2	5	22.2073	21.5537	-21.4952	-1.5881	0.6535
-11	3	5	85.9765	87.9423	-87.8931	-2.9424	-1.9659
5	3	5	6.7048	5.3496	-4.9715	1.9755	1.3551
7	3	5	27.2548	25.8530	-25.8175	-1.3539	1.4018
-12	4	5	7.3904	7.7688	-7.7622	-0.3210	-0.3784
-10	4	5	17.8308	18.2130	18.1543	1.4619	-0.3823
6	4	5	59.2195	57.9327	-57.9022	-1.8792	1.2868
-11	5	5	46.5537	46.8602	-46.8045	-2.2857	-0.3065
5	5	5	39.6818	38.9116	38.8439	2.2943	0.7701
7	5	5	8.9159	9.2159	9.1649	-0.9684	-0.3000
-12	6	5	23.6442	24.4207	24.4207	0.0227	-0.7765
-10	6	5	59.6990	60.6541	60.6302	1.7040	-0.9551
6	6	5	14.1982	13.8229	-13.7540	-1.3785	0.3752
-11	7	5	5.3244	4.5104	-4.0695	-1.9449	0.8140
-9	7	5	10.6746	11.0895	10.9668	1.6451	-0.4149
5	7	5	25.3347	24.4308	24.3513	1.9693	0.9039
-10	8	5	20.1622	20.7793	-20.7678	0.6934	-0.6171
4	8	5	26.3703	25.7468	-25.7464	0.1480	0.6234
6	8	5	12.4897	12.0756	12.0262	-1.0912	0.4141
-11	9	5	14.3788	13.8965	-13.7790	-1.8028	0.4823
-9	9	5	16.8220	17.0530	-17.0098	1.2131	-0.2310
3	9	5	36.5232	36.8453	-36.7698	-2.3576	-0.3221
5	9	5	16.9951	15.9711	15.8727	1.7697	1.0240
-10	10	5	20.2178	20.6545	20.6189	1.2120	-0.4367
-8	10	5	8.9528	8.2400	8.0843	-1.5942	0.7129
4	10	5	5.3340	5.5849	5.5543	0.5833	-0.2509
6	10	5	9.4472	8.3156	-8.2542	-1.0091	1.1316
-9	11	5	48.3331	49.2177	49.1770	2.0029	-0.8847
-7	11	5	13.4373	12.7545	12.7405	-0.5968	0.6829
3	11	5	6.9291	7.2356	-6.9537	-2.0001	-0.3065
5	11	5	26.2500	26.0153	25.9503	1.8387	0.2347
-10	12	5	24.3941	25.0811	25.0505	1.2375	-0.6870
-8	12	5	32.0466	32.4813	-32.4234	-1.9380	-0.4347
-6	12	5	57.3328	55.7758	55.7091	2.7266	1.5570
0	12	5	25.2909	23.4106	-23.3841	-1.1143	1.8803
2	12	5	4.5926	4.7525	-4.7512	0.1086	-0.1599
4	12	5	34.1210	36.4657	36.4539	0.9302	-2.3448
-9	13	5	29.2486	30.3224	30.2872	1.4611	-1.0738
-7	13	5	25.9730	25.7816	-25.7556	-1.1569	0.1914
-5	13	5	24.0162	23.2819	-23.2787	-0.3855	0.7343
-3	13	5	26.0100	24.4542	24.4324	1.0334	1.5558
-1	13	5	76.8584	75.0264	-74.9904	-2.3246	1.8320
1	13	5	45.0395	44.9578	44.9031	2.2184	0.0817
3	13	5	52.2058	52.4674	-52.4154	-2.3352	-0.2616
-8	14	5	62.4176	64.2649	-64.2303	-2.1086	-1.8473
-6	14	5	23.8947	22.5456	22.4612	1.9486	1.3491

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-4	14	5	63.3899	58.0380	-57.9807	-2.5798	5.3516
-2	14	5	7.0042	7.0484	6.8749	1.5544	-0.0442
0	14	5	25.3125	24.5483	-24.5164	-1.2505	0.7642
2	14	5	16.0992	16.9585	-16.9582	-0.1014	-0.8593
-7	15	5	10.4825	8.5215	-8.4916	-0.7141	1.9610
-5	15	5	8.8507	8.0957	8.0957	0.0180	0.7551
-3	15	5	4.7419	4.6211	-4.5605	0.7464	0.1208
-1	15	5	10.3581	8.6295	-8.5168	-1.3897	1.7286
1	15	5	35.5605	34.5279	34.4808	1.8031	1.0326
-6	16	5	30.7243	30.7538	30.7023	1.7789	-0.0295
-4	16	5	20.6510	20.4931	20.4549	-1.2498	0.1580
-2	16	5	27.7618	28.0865	28.0379	1.6509	-0.3247
0	16	5	2.1261	3.1766	3.0950	-0.7154	-1.0505
-5	17	5	16.5882	16.2602	16.2573	0.3098	0.3280
-3	17	5	5.4604	6.2673	-6.2398	0.5871	-0.8069
-1	17	5	21.5510	24.5724	24.5632	-0.6726	-3.0214
-12	0	6	38.3632	38.7202	-38.6626	-2.1109	-0.3570
-10	0	6	69.7163	70.8384	70.7766	2.9600	-1.1221
4	0	6	35.6923	35.0708	34.9978	2.2627	0.6215
6	0	6	67.2464	63.9447	-63.8949	-2.5232	3.3017
-11	1	6	20.8509	21.4879	-21.4629	-1.0358	-0.6370
5	1	6	20.0691	19.4915	-19.4905	0.1947	0.5776
-12	2	6	25.2997	26.3765	-26.3093	-1.8818	-1.0768
-10	2	6	32.2349	31.8017	31.6988	2.5562	0.4333
4	2	6	53.6887	50.9392	50.8812	2.4307	2.7495
6	2	6	18.3272	16.8335	-16.7233	-1.9230	1.4937
-11	3	6	0.0000	0.8142	-0.1891	-0.7919	-0.8142
5	3	6	46.5278	44.7281	44.7171	0.9916	1.7997
-12	4	6	3.6366	2.1262	-1.4937	-1.5131	1.5104
-10	4	6	5.7352	7.3679	-7.0864	2.0170	-1.6326
4	4	6	4.6018	3.5097	2.9751	1.8619	1.0921
6	4	6	12.8207	11.1242	-10.9667	-1.8653	1.6965
-11	5	6	0.0000	0.7916	-0.3105	-0.7282	-0.7916
-9	5	6	0.0000	0.8391	0.8379	-0.0449	-0.8391
3	5	6	61.5023	58.8588	-58.8285	-1.8897	2.6435
5	5	6	17.8596	15.9141	15.9043	0.5584	1.9456
-12	6	6	14.7702	12.9647	-12.8661	-1.5957	1.8056
-10	6	6	26.1024	26.3539	26.2584	2.2418	-0.2515
4	6	6	4.1355	2.9266	2.3561	1.7361	1.2088
6	6	6	41.1466	38.8510	-38.7929	-2.1233	2.2956
-11	7	6	11.7382	11.8123	-11.7804	-0.8668	-0.0741
-9	7	6	15.3867	16.7804	16.7804	-0.0005	-1.3936
3	7	6	0.0000	1.2665	-0.0342	-1.2661	-1.2665
5	7	6	3.3942	4.0847	-4.0674	0.3765	-0.6905
-10	8	6	52.7170	53.2983	53.2363	2.5700	-0.5813
-8	8	6	45.3125	45.6196	-45.5409	-2.6790	-0.3071
2	8	6	9.6255	8.8010	-8.6490	-1.6283	0.8245
4	8	6	74.0228	71.4315	71.3888	2.4719	2.5913
-11	9	6	19.3516	20.7071	-20.6865	-0.9249	-1.3556
-9	9	6	5.8886	3.9107	-3.9094	-0.0989	1.9779
-7	9	6	40.7316	39.8793	39.8567	1.3445	0.8523
1	9	6	36.5397	34.4147	34.3393	2.2771	2.1250
3	9	6	4.5273	4.2176	4.0927	-1.0187	0.3097
5	9	6	0.0000	2.7034	-2.6830	0.3319	-2.7034
-10	10	6	23.6298	23.8654	23.7720	2.1097	-0.2356

h	k	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-8	10	6	54.2003	53.6217	-53.5656	-2.4524	0.5787
0	10	6	6.2254	6.6954	6.6539	0.7442	-0.4700
2	10	6	52.4975	51.7128	-51.6827	-1.7628	0.7847
4	10	6	20.2137	19.1993	19.1193	1.7515	1.0144
-9	11	6	7.6333	8.1256	-8.1251	-0.0881	-0.4923
-7	11	6	0.0000	1.0196	0.6477	0.7875	-1.0196
-5	11	6	24.7914	22.5750	-22.5056	-1.7693	2.2163
-1	11	6	28.0387	27.6768	-27.5725	-2.4008	0.3620
1	11	6	9.3929	9.2997	9.1494	1.6651	0.0932
3	11	6	47.4975	46.0474	-46.0222	-1.5227	1.4501
-8	12	6	10.8378	10.0057	-9.8608	-1.6966	0.8321
-6	12	6	16.7001	15.7558	15.6775	1.5696	0.9443
-4	12	6	17.9975	15.8309	-15.7891	-1.1494	2.1666
-2	12	6	0.0000	1.1703	1.1208	0.3366	-1.1703
0	12	6	11.5003	12.4579	-12.4548	0.2774	-0.9576
2	12	6	0.0000	1.3555	0.8614	-1.0466	-1.3555
-9	13	6	12.5844	13.7649	13.7646	0.0849	-1.1804
-7	13	6	11.0723	11.46	-11.4441	0.6244	-0.3888
-5	13	6	14.0070	13.8792	13.8364	-1.0901	0.1278
-3	13	6	4.6672	4.0962	3.7046	1.7478	0.5710
-1	13	6	3.7206	2.6622	-2.0740	-1.6691	1.0583
1	13	6	29.1969	27.0577	26.9983	1.7919	2.1393
3	13	6	19.3973	18.6114	-18.5810	-1.0635	0.7859
-8	14	6	4.3778	1.5657	-0.4545	-1.4983	2.8121
-6	14	6	22.0017	21.3915	21.3370	1.5260	0.6102
-4	14	6	12.0882	12.8531	12.8277	-0.8076	-0.7649
-2	14	6	26.7806	27.2105	27.2057	0.5150	-0.4300
0	14	6	9.6867	9.0212	9.0037	0.5620	0.6656
2	14	6	28.8616	29.6640	29.6566	-0.6618	-0.8023
-7	15	6	10.8522	10.1054	10.0777	0.7472	0.7468
-5	15	6	22.9860	22.8204	-22.7745	-1.4457	0.1656
-3	15	6	42.6722	41.0685	41.0257	1.8739	1.6037
-1	15	6	17.7661	17.9567	-17.8648	-1.8147	-0.1906
1	15	6	21.9939	18.9360	18.8763	1.5029	3.0579
-4	16	6	28.7740	28.1612	-28.1427	-1.0225	0.6128
-2	16	6	21.8841	23.8977	-23.8972	-0.1465	-2.0136
-12	0	7	39.2282	39.9322	-39.8752	-2.1320	-0.7039
-10	0	7	27.6123	28.3103	-28.2825	1.2529	-0.6980
2	0	7	34.4822	33.2875	-33.1873	-2.5808	1.1948
4	0	7	11.0849	8.8515	8.6770	1.7490	2.2334
-11	1	7	6.6909	6.1967	-6.1577	0.6943	0.4942
-9	1	7	5.9498	6.6232	-6.3721	-1.8066	-0.6735
3	1	7	24.3012	22.6343	-22.6343	0.0308	1.6669
5	1	7	5.5949	3.6495	-3.5156	-0.9796	1.9454
-12	2	7	6.1871	4.9871	-4.6591	-1.7786	1.2001
-10	2	7	50.6015	51.9770	51.9302	2.2047	-1.3755
2	2	7	20.3462	18.8096	-18.6788	-2.2144	1.5366
4	2	7	32.8257	29.6085	29.5309	2.1427	3.2171
-11	3	7	45.0692	45.5593	45.5359	1.4615	-0.4901
-9	3	7	37.1756	37.6934	-37.6493	-1.8233	-0.5179
3	3	7	52.5912	49.0965	49.0871	0.9604	3.4947
5	3	7	6.0847	5.1652	-5.0596	-1.0392	0.9195
-12	4	7	40.9576	43.0817	-43.0193	-2.3193	-2.1241
-10	4	7	39.1893	39.1892	39.1296	2.1602	0.0001
2	4	7	56.8463	52.7881	-52.7260	-2.5589	4.0582

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
4	4	7	25.1902	21.5929	21.5081	1.9114	3.5973
-11	5	7	10.4223	9.4254	9.3905	0.8109	0.9969
-9	5	7	79.7007	79.9804	-79.9402	-2.5361	-0.2797
1	5	7	57.8868	53.4711	-53.4710	-0.0650	4.4158
3	5	7	8.5385	8.1790	8.1665	0.4520	0.3595
-10	6	7	0.0000	1.6306	-0.5860	1.5217	-1.6306
-8	6	7	39.1290	39.4913	-39.4610	-1.5463	-0.3624
2	6	7	52.9170	49.1689	-49.1020	-2.5643	3.7481
4	6	7	13.7265	11.3142	11.1967	1.6266	2.4122
-11	7	7	6.1455	7.0098	6.9560	0.8673	-0.8643
-9	7	7	3.2310	3.5521	3.2378	-1.4609	-0.3211
-7	7	7	19.9776	19.4517	19.3207	2.2534	0.5259
1	7	7	32.3149	28.6916	28.6319	0.7474	3.6233
3	7	7	8.1605	7.7259	7.7193	0.3198	0.4346
-10	8	7	43.1959	45.1328	45.0948	1.8532	-1.9369
-8	8	7	39.4244	39.6420	39.6376	-0.5892	-0.2176
0	8	7	38.2777	37.1437	37.0809	2.1587	1.1340
2	8	7	10.3117	9.6742	9.5362	-1.6281	0.6375
4	8	7	31.6660	28.9844	28.9176	1.9669	2.6816
-9	9	7	16.3589	17.1186	17.0860	-1.0550	-0.7596
-7	9	7	7.4277	5.3324	4.9401	2.0076	2.0952
-5	9	7	21.7891	20.6642	20.5861	-1.7942	1.1249
-3	9	7	33.1124	38.5965	38.5344	2.1879	-5.4841
-1	9	7	17.8136	18.2701	-18.2255	-1.2762	-0.4566
1	9	7	47.2713	44.0981	44.0878	0.9503	3.1733
3	9	7	9.5504	8.1884	-8.1865	0.1783	1.3619
-10	10	7	5.6515	7.9452	-7.8525	1.2101	-2.2936
-8	10	7	39.2993	39.7133	-39.6935	-1.2548	-0.4140
-6	10	7	13.7459	13.7540	-13.7538	0.0561	-0.0081
-4	10	7	31.5557	31.0431	-31.0414	0.3179	0.5126
-2	10	7	31.8139	33.6722	-33.6361	-1.5598	-1.8583
0	10	7	8.0206	7.1433	6.9556	1.6267	0.8774
2	10	7	32.5248	30.2454	-30.1771	-2.0317	2.2794
-9	11	7	55.2853	56.8038	-56.7696	-1.9702	-1.5185
-7	11	7	8.6459	8.4062	8.2259	1.7317	0.2397
-5	11	7	64.4394	62.0880	-62.0314	-2.6514	2.3513
-3	11	7	6.3416	6.3492	-6.1637	1.5237	-0.0076
-1	11	7	46.0830	45.3910	-45.3629	-1.5981	0.6919
1	11	7	33.8750	32.6458	-32.6458	-0.0064	1.2292
-8	12	7	17.9580	18.0259	-17.9932	-1.0858	-0.0679
-6	12	7	11.0277	11.6585	-11.6584	-0.0486	-0.6308
-4	12	7	9.4158	8.8232	8.7885	0.7817	0.5926
-2	12	7	44.5562	46.0920	-46.0567	-1.8030	-1.5358
0	12	7	37.1874	35.7977	35.7446	1.9466	1.3897
-7	13	7	67.5531	67.3246	67.2796	2.4612	0.2285
-5	13	7	32.9665	32.5867	-32.5266	-1.9783	0.3798
-3	13	7	50.1702	56.5277	56.4879	2.1194	-6.3574
-1	13	7	13.2183	14.8943	14.8757	-0.7437	-1.6760
1	13	7	3.8510	1.0687	-1.0107	0.3475	2.7823
-6	14	7	22.4147	22.1764	22.1722	0.4325	0.2382
-4	14	7	43.5290	44.7487	44.7350	1.1074	-1.2197
-2	14	7	0.0000	1.7313	1.3588	-1.0728	-1.7313
-5	15	7	12.3461	10.5405	-10.4141	-1.6276	1.8056
-12	0	8	14.1177	16.3690	-16.3264	-1.1799	-2.2513
-10	0	8	17.9994	20.1435	-20.1435	-0.0485	-2.1441

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-8	0	8	42.5445	41.7901	41.7762	1.0778	0.7544
0	0	8	63.4782	60.2529	60.2049	2.4044	3.2253
2	0	8	4.3596	4.5879	-4.4351	-1.1818	-0.2284
-11	1	8	41.1023	42.7671	42.7051	2.3018	-1.6648
-9	1	8	64.8107	65.3215	-65.2650	-2.7155	-0.5109
1	1	8	43.4205	40.4624	-40.4324	-1.5584	2.9581
3	1	8	45.4308	40.5119	40.4634	1.9805	4.9190
-12	2	8	6.2712	5.6432	-5.5771	-0.8616	0.6280
-10	2	8	9.8644	11.4079	11.4049	0.2651	-1.5435
-8	2	8	13.4538	12.3613	12.3314	0.8589	1.0925
0	2	8	16.5655	15.3084	15.1664	2.0801	1.2571
2	2	8	36.0347	31.2152	-31.1760	-1.5633	4.8195
-11	3	8	11.0807	10.3027	10.1285	1.8862	0.7780
-9	3	8	4.4618	2.0202	-0.3643	-1.9871	2.4416
-7	3	8	11.0506	10.5621	10.3637	2.0376	0.4885
-1	3	8	35.8294	35.6330	-35.6328	0.1042	0.1964
1	3	8	8.2165	7.1865	7.0991	-1.1174	1.0300
3	3	8	4.9887	2.8529	2.4931	1.3869	2.1358
-10	4	8	21.0620	22.1412	22.1387	0.3331	-1.0792
-8	4	8	20.3001	20.7913	-20.7862	0.4583	-0.4911
0	4	8	16.5132	14.9647	14.8254	2.0370	1.5485
2	4	8	28.5014	24.7608	-24.7096	-1.5911	3.7406
-11	5	8	6.4208	7.1818	-7.0223	1.5054	-0.7610
-9	5	8	11.0910	10.7206	-10.5319	-2.0026	0.3703
-7	5	8	0.0000	1.8245	-0.0261	1.8243	-1.8245
-1	5	8	35.6928	35.0224	-35.0221	0.1427	0.6704
1	5	8	19.1680	18.4216	18.4047	-0.7904	0.7464
3	5	8	12.3370	10.9182	10.8121	1.5184	1.4188
-10	6	8	0.0000	2.1598	-2.1574	0.1015	-2.1598
-8	6	8	0.0000	4.4538	4.4117	0.6115	-4.4538
-6	6	8	7.8530	7.5730	-7.4221	-1.5042	0.2800
-4	6	8	26.6078	27.8468	27.7651	2.1317	-1.2390
-2	6	8	6.2248	5.9771	-5.5690	-2.1705	0.2478
0	6	8	43.0501	41.3918	41.3370	2.1293	1.6583
2	6	8	14.1217	12.7035	-12.6385	-1.2836	1.4183
-9	7	8	43.9462	45.6095	-45.5515	-2.2979	-1.6633
-7	7	8	61.1331	59.6429	59.6045	2.1382	1.4902
-5	7	8	12.6287	13.1100	-13.0411	-1.3429	-0.4814
-3	7	8	4.6534	5.7206	-5.7096	0.3547	-1.0672
-1	7	8	38.4063	39.7983	39.7926	0.719	-1.3919
1	7	8	27.8981	27.5470	-27.5137	0.3533	0.3511
-10	8	8	0.0000	0.6947	-0.6746	0.1658	-0.6947
-8	8	8	34.9703	35.6787	35.6635	1.0437	-0.7085
-6	8	8	44.4498	44.7059	-44.6667	-1.8702	-0.2560
-4	8	8	34.6632	35.7188	35.6408	2.3581	-1.0556
-2	8	8	41.8192	44.3941	-44.3252	-2.4733	-2.5749
0	8	8	18.1212	16.8368	16.7394	1.8079	1.2844
2	8	8	32.9194	29.2637	-29.2351	-1.2930	3.6558
-9	9	8	44.4625	45.7535	-45.6990	-2.2311	-1.2910
-7	9	8	47.5201	46.1805	46.1346	2.0578	1.3396
-5	9	8	13.5990	13.3607	-13.3039	-1.2302	0.2383
-3	9	8	15.6912	18.0293	-18.0284	0.1780	-2.3381
-1	9	8	28.9773	30.0776	30.0692	0.7128	-1.1003
1	9	8	43.2324	41.2548	-41.2275	-1.5005	1.9776
-8	10	8	10.2891	10.6347	10.6100	0.7239	-0.3456

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-6	10	8	37.3232	38.9425	-38.9098	-1.5960	-1.6193
-4	10	8	43.7184	47.4931	47.4462	2.1098	-3.7748
-2	10	8	28.8790	28.9482	-28.8731	-2.0849	-0.0693
0	10	8	26.5286	24.0382	23.9718	1.7860	2.4903
-7	11	8	3.4549	3.2720	-2.9147	1.4869	0.1829
-5	11	8	17.3477	17.4829	-17.4437	-1.1706	-0.1352
-3	11	8	5.9030	5.7453	5.7235	0.5002	0.1577
-1	11	8	19.1758	19.5526	-19.5508	0.2647	-0.3768
-6	12	8	5.4133	4.7785	-4.6801	-0.9646	0.6348
-4	12	8	7.7129	7.9334	7.8064	1.4135	-0.2205
-2	12	8	12.3507	11.6332	-11.5223	-1.6024	0.7175
-5	13	8	6.3644	4.5149	-4.3973	-1.0236	1.8495
-3	13	8	21.9409	23.5961	23.5887	0.5898	-1.6552
-10	0	9	43.5313	47.5425	47.5384	-0.6266	-4.0112
-8	0	9	34.2761	34.4746	34.4111	2.0921	-0.1985
-6	0	9	38.3551	40.4576	40.4282	-1.5418	-2.1025
-4	0	9	70.0054	77.2541	77.2123	2.5394	-7.2486
-2	0	9	0.0000	1.2699	-0.3250	-1.2276	-1.2699
0	0	9	58.4562	56.7768	56.7603	1.3686	1.6794
-11	1	9	18.8428	18.8398	18.7667	1.6574	0.0030
-9	1	9	0.0000	1.5700	1.1697	-1.0413	-1.5700
-7	1	9	29.3757	29.1970	29.1868	0.7714	0.1727
-5	1	9	4.0002	0.6473	0.5090	0.3998	3.3529
-3	1	9	21.9013	23.0961	23.0809	-0.8389	-1.1948
-1	1	9	19.5590	19.9528	19.8726	1.7867	-0.3938
1	1	9	0.0000	3.2943	2.8481	-1.6555	-3.2943
-10	2	9	38.7810	40.7700	-40.7360	-1.6650	-1.9891
-8	2	9	5.9729	5.1092	-4.8157	1.7067	0.8637
-6	2	9	55.1412	58.3397	-58.2818	-2.6002	-3.1985
-4	2	9	3.8745	4.1752	3.7652	1.8041	-0.3006
-2	2	9	43.0933	44.4482	-44.4116	-1.8040	-1.3549
0	2	9	11.5631	12.1111	-12.1041	0.4136	-0.5481
-11	3	9	6.9008	5.5943	5.4001	1.4611	1.3065
-9	3	9	37.3116	37.3984	-37.3642	-1.5988	-0.0867
-7	3	9	27.1280	27.1459	-27.1459	-0.0560	-0.0179
-5	3	9	16.9564	18.2201	-18.2183	0.2619	-1.2637
-3	3	9	67.6530	72.9009	-72.8736	-1.9959	-5.2479
-1	3	9	12.1005	13.3174	13.2151	1.6470	-1.2169
1	3	9	66.3686	64.1570	-64.1124	-2.3916	2.2116
-10	4	9	48.3939	50.2498	-50.2175	-1.8007	-1.8560
-8	4	9	46.5562	47.5253	47.4675	2.3429	-0.9691
-6	4	9	54.7958	57.4442	-57.3854	-2.6001	-2.6484
-4	4	9	21.6504	23.3596	23.2667	2.0816	-1.7092
-2	4	9	13.7186	13.0398	-12.9675	-1.3715	0.6788
0	4	9	20.0608	20.6909	-20.6889	0.2915	-0.6301
-9	5	9	0.0000	1.2415	-0.8616	-0.8938	-1.2415
-7	5	9	16.5764	16.5010	16.4895	0.6158	0.0754
-5	5	9	45.1130	49.1082	49.0953	1.1239	-3.9952
-3	5	9	20.7370	22.7108	-22.6751	-1.2722	-1.9737
-1	5	9	73.3611	75.3733	75.3346	2.4146	-2.0122
1	5	9	11.8218	8.8762	-8.7232	-1.6412	2.9455
-10	6	9	4.5973	4.7793	4.6528	-1.0924	-0.1820
-8	6	9	53.0864	54.1342	54.0841	2.3275	-1.0477
-6	6	9	5.9354	4.4530	4.0545	-1.8413	1.4824
-4	6	9	57.2767	62.4408	62.3962	2.3582	-5.1641

H	K	L	F(OBS)	F(CALC)	A	B	OBS-CALC
-2	6	9	6.1549	6.6650	6.5849	-1.0300	-0.5101
0	6	9	26.3650	25.0350	25.0205	0.8528	1.3300
-9	7	9	10.5497	9.4938	-9.4239	-1.1494	1.0559
-7	7	9	11.0581	10.1985	10.1898	0.4213	0.8596
-5	7	9	4.1682	3.8997	-3.8938	0.2133	0.2686
-3	7	9	4.0984	5.2284	-5.1145	-1.0855	-1.1300
-1	7	9	7.9408	6.5133	6.3537	1.4327	1.4275
-8	8	9	32.5737	36.0899	-36.0761	0.9958	-3.5161
-6	8	9	34.8874	38.5662	-38.5067	-2.1426	-3.6789
-4	8	9	5.3338	3.7542	-3.4989	1.3608	1.5796
-2	8	9	49.8455	54.3877	-54.3571	-1.8222	-4.5422
0	8	9	4.0188	0.6416	-0.4246	0.4810	3.3773
-7	9	9	0.0000	1.0303	0.9781	0.3240	-1.0303
-5	9	9	35.3862	39.3313	-39.3309	-0.1768	-3.9451
-3	9	9	0.0000	0.9990	-0.2973	-0.9538	-0.9990
-1	9	9	15.1567	17.6099	-17.5806	1.0158	-2.4532
-6	10	9	4.0283	3.7320	-3.4072	-1.5227	0.2963
-4	10	9	29.1741	32.3474	32.2948	1.8437	-3.1733
-2	10	9	6.6208	5.1375	-5.0292	-1.0492	1.4833
-5	11	9	20.6076	23.0529	23.0387	0.8087	-2.4453
-8	0	10	36.5121	39.2602	39.2009	2.1578	-2.7481
-6	0	10	4.9611	5.9145	5.8088	-1.1131	-0.9534
-4	0	10	4.5970	1.6481	-1.5767	0.4800	2.9488
-2	0	10	16.8826	17.9058	17.8966	0.5757	-1.0232
-9	1	10	27.2150	29.2333	29.2233	0.7661	-2.0184
-7	1	10	30.6504	34.4776	-34.4471	-1.4501	-3.8273
-5	1	10	52.1796	59.0895	59.0502	2.1544	-6.9099
-3	1	10	27.3850	29.7157	-29.6426	-2.0836	-2.3307
-1	1	10	27.2303	26.8872	26.8269	1.8002	0.3430
-8	2	10	16.5954	17.3705	17.2878	1.6931	-0.7751
-6	2	10	16.4373	18.5961	-18.5404	-1.4388	-2.1588
-4	2	10	0.0000	1.2132	1.0931	0.5263	-1.2132
-2	2	10	3.7159	3.7647	3.7605	0.1782	-0.0488
-9	3	10	24.5778	26.2832	-26.2832	0.0077	-1.7054
-7	3	10	12.7585	13.5856	-13.5388	-1.1275	-0.8271
-5	3	10	19.7248	22.3848	-22.3460	1.3167	-2.6599
-3	3	10	21.9725	23.4519	-23.3747	-1.9013	-1.4794
-1	3	10	11.2119	11.3328	11.2084	1.6746	-0.1209
-8	4	10	16.3533	17.8067	17.7346	1.6009	-1.4533
-6	4	10	26.3901	29.3793	-29.3446	-1.4276	-2.9893
-4	4	10	12.4127	14.1988	14.1747	0.8261	-1.7861
-2	4	10	18.9156	19.5585	-19.5577	-0.1846	-0.6430
-7	5	10	18.5219	21.7832	21.7739	-0.6364	-3.2614
-5	5	10	6.6397	6.2723	6.0955	1.4788	0.3674
-3	5	10	6.3883	7.9876	7.8336	-1.5608	-1.5993
-8	6	10	26.0697	28.6371	28.5807	1.7957	-2.5674
-6	6	10	6.8079	7.4660	-7.3780	-1.1429	-0.6581
-4	6	10	17.1391	18.2350	18.2199	0.7418	-1.0959
-7	7	10	29.6100	34.0078	-33.9822	-1.3183	-4.3978
-5	7	10	33.4268	38.2018	38.1613	1.7573	-4.7750
-3	7	10	26.1082	28.6388	-28.5774	-1.8755	-2.5307

	R(F)	R(F**2)

ALL INTENSITIES (1367 REFLECTIONS)

	R(F)	R(F**2)
RATIO	0.0498	0.0802
NUMERATOR	0.226272046E 04	0.212429392E 06
DENOMINATOR	0.454116174E 05	0.264740126E 07

GREATER THAN YMIN = 0.00 (1319 REFLECTIONS)

	R(F)	R(F**2)
RATIO	0.0478	0.0802
NUMERATOR	0.217205013E 04	0.212213745E 06
DENOMINATOR	0.454116174E 05	0.264740126E 07