

## The crystal structure of an Al-rich titanite from Grisons, Switzerland

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### Abstract

The structure of an Al-rich titanite has been refined in several space groups to provide data on a natural titanite and to evaluate the structural effects of the coupled substitution  $(\text{Al,Fe})^{3+} + (\text{OH,F})^{-} = \text{Ti}^{4+} + \text{O}^{2-}$ . Titanite from Grisons, Switzerland,  $\text{Ca}(\text{Ti}_{0.90}\text{Al}_{0.09}\text{Fe}_{0.01}^{3+})\text{O}_{0.98}\text{SiO}_{3.96}(\text{OH}_{0.08}\text{F}_{0.02})$ , is monoclinic with  $a = 7.050(3)$ ,  $b = 8.681(4)$ , and  $c = 6.539(2)\text{\AA}$  and  $\beta = 113.90(3)^{\circ}$ . Anisotropic refinement in space group  $A2/a$  ( $R_w = 0.048$ ) yielded results similar to those obtained by Mongiorgi and di Sanseverino (1968) for titanite from Zillertal except that the mean Ti-O bond length is smaller due to substitution of Al for Ti in the octahedral site. The orientation of the maximum thermal vibrational displacement for most atoms subparallel to  $a$  reflects positional disordering due to the development of a domain texture. The details of the  $P2_1/a$  refinement ( $R_w = 0.065$ ) are comparable to those of synthetic  $P2_1/a$  titanite (Speer and Gibbs, 1976). Despite extensive  $\text{Al}^{3+} \rightarrow \text{Ti}^{4+}$  substitution, the alternating long and short Ti-O(1) bond lengths, (1.970 and 1.768\AA, Fig. 1) which reflect the amount of displacement of the Ti atom from the geometric center of the Ti octahedron are the same as for the synthetic  $P2_1/a$  titanite at 25°C (Taylor and Brown, 1976). The extreme distortion of some of the Si and Ti polyhedra and unreasonable bond distances cast doubt on the reliability of refinement in space group  $P2_1$  constrained by only 21 weak maxima of type  $h0l$ ,  $h = \text{odd}$ . The weak maxima are the result of diffuse  $h$ -relplanes. It is possible that the  $h$ -relplanes are due either to linear positional ordering or to chemical cation ordering in the octahedral sites.

### Introduction

The space group of synthetic titanite,  $\text{CaTiOSiO}_4$ , is  $P2_1/a$  (Robbins, 1968; Speer and Gibbs, 1976), the diffraction pattern showing sharp but weak  $k + l = \text{odd}$  reflections in violation of the A-centering of the previously reported space group  $A2/a$  of natural titanites (Zachariasen, 1930; Mongiorgi and di Sanseverino, 1968). Refinement of the structure (Speer and Gibbs, 1976) showed that the sharp but weak  $k + l = \text{odd}$  reflections are due to displacement of the Ti atoms from the geometric centers of the octahedra.

The observation of diffuse  $k + l = \text{odd}$  reflections on long exposure single crystal photographs of natural titanites led Speer and Gibbs (1976) to conclude that the

structure of stoichiometric synthetic titanite consists essentially of a single domain of  $P2_1/a$  symmetry while that of natural titanite consists of a large and variable number of  $P2_1/a$  domains related to one another by half turn parallel to  $b$ . This brings all atoms in two neighboring domains into coincidence except Ti which in effect is linearly disordered, resulting in the observed diffuse streaking of the  $k + l = \text{odd}$  reflections. Out-of-step linear domain formation in natural titanites appears to be favored by the substitution,  $(\text{Al,Fe})^{3+} + (\text{OH,F})^{-} = \text{Ti}^{4+} + \text{O}^{2-}$ , with the  $k + l = \text{odd}$  reflections becoming unobservable above ~ 20 mole percent substituents (Higgins and Ribbe, 1976). The quasi-mirror displacement of the "Ti" atoms either towards or away from the domain boundaries (Fig. 4 in Taylor and Brown, 1976) provides the necessary charge balance at the sites of  $\text{R}^{3+}$  and  $\text{OH/F}$  substitution, respectively. The present study was undertaken to determine the effects of extensive  $\text{Al}^{3+}$  for  $\text{Ti}^{4+}$  substitution on the titanite structure.

<sup>1</sup> To obtain a copy of Table I, order document AM-84-240 from the Business Office, Mineralogical Society of America, 2000 Florida Ave., N.W., Washington, DC 20009. Please remit \$5.00 in advance for microfiche.

A2/a	h	k	l	F(obs)	F(calc)	SF*	A2/a	h	k	l	F(obs)	F(calc)	SF*
0	-16	4		45.8760	45.7443	1							
0	-16	2		31.4950	28.5216	1	1	-1	7		49.2100	49.0394	1
0	-16	0		48.5840	45.0807	1	1	-1	5		33.6400	33.6402	1
0	-15	1		84.3690	85.7614	1	1	-2	4		26.5980	29.6813	1
0	-15	3		95.5990	92.0346	1	1	-3	11		22.1890	16.8749	1
0	-15	5		57.8730	51.9971	1	1	-3	7		30.7040	30.3030	1
0	-14	4		20.6800	11.0645	1	1	-3	5		16.8040	18.4200	1
0	-14	0		40.1500	36.7062	1	1	-3	3		83.5310	78.0985	1
0	-13	1		49.8800	48.9501	1	1	-4	2		33.4480	31.8157	1
0	-13	3		63.8120	64.2300	1	1	-4	4		55.6760	56.4030	1
0	-13	5		40.7490	36.8445	1	1	-4	8		17.0920	2.1910	1
0	-13	7		43.2970	42.5404	1	1	-4	10		43.8380	46.2947	1
0	-12	8		63.7470	55.4119	1	1	-5	9		27.4560	23.9572	1
0	-12	6		107.5030	107.8244	1	1	-5	7		16.4440	12.0084	1
0	-12	4		126.0070	121.7363	1	1	-5	5		33.2330	33.3416	1
0	-12	2		102.6260	103.1314	1	1	-5	3		22.7960	15.7353	1
0	-12	0		104.1790	100.9405	1	1	-5	1		15.7130	9.3362	1
0	-11	1		20.4480	18.1084	1	1	-6	2		23.7320	24.9401	1
0	-10	8		45.7930	46.6585	1	1	-6	4		58.5890	57.9679	1
0	-10	4		28.3740	27.6474	1	1	-6	6		53.4970	50.3056	1
0	-10	2		63.1030	62.8657	1	1	-6	8		26.3680	17.9604	1
0	-10	0		62.3840	58.1209	1	1	-8	2		15.3920	14.8052	1
0	-9	1		168.0850	177.3751	1	1	-8	4		53.8310	52.7307	1
0	-9	3		107.8790	104.1410	1	1	-8	6		54.9590	56.1301	1
0	-9	5		115.6070	115.2487	1	1	-8	8		36.5430	35.8399	1
0	-9	7		92.8030	89.7219	1	1	-8	10		21.2650	16.8020	1
0	-9	9		84.8460	84.0662	1	1	-9	7		18.1120	7.2858	1
0	-8	6		23.1630	28.8077	1	1	-9	5		17.8000	18.4764	1
0	-8	2		15.0600	10.1263	1	1	-9	3		30.9430	26.6888	1
0	-8	0		87.4740	86.0918	1	1	-9	1		32.3620	33.3335	1
0	-7	1		14.7880	15.4026	1	1	-10	6		28.3690	20.8893	1
0	-7	3		17.8920	10.8475	1	1	-10	8		18.0720	20.0671	1
0	-7	5		85.9910	82.5918	1	1	-11	7		45.4490	43.8021	1
0	-6	10		72.4030	73.3140	1	1	-11	3		68.6920	68.1964	1
0	-6	8		124.9100	124.3214	1	1	-11	1		98.4120	94.9466	1
0	-6	6		119.9820	118.5389	1	1	-12	2		49.6700	45.4505	1
0	-6	4		161.3920	167.5619	1	1	-13	5		17.9720	14.2702	1
0	-6	0		157.0100	158.7323	1	1	-13	3		19.2380	21.3648	1
0	-5	3		65.0450	60.1567	1	1	-13	1		29.2860	28.5239	1
0	-5	5		26.8850	31.6196	1	1	-14	2		31.5590	30.7097	1
0	-5	7		21.7690	17.2380	1	1	-14	4		48.7680	46.5911	1
0	-5	11		19.8480	20.1743	1	1	-14	6		37.5120	39.1425	1
0	-4	10		27.5440	28.8595	1	1	-15	5		38.7450	31.3140	1
0	-4	8		35.5470	30.8635	1	1	-15	3		27.8000	17.6576	1
0	-4	6		19.3590	13.6561	1	1	-17	1		31.1150	17.9043	1
0	-4	4		17.8720	14.8817	1	2	-16	2		43.5040	38.2421	1
0	-3	5		209.9180	216.8841	1	2	-15	1		35.8370	32.0291	1
0	-3	7		158.3290	157.7925	1	2	-14	4		43.4800	43.2084	1
0	-3	9		111.1960	108.1865	1	2	-14	2		63.7740	61.9606	1
0	-3	11		73.3220	76.6842	1	2	-13	1		30.6550	19.8987	1
0	-2	6		57.9790	57.1250	1	2	-13	3		43.2860	40.8720	1
0	-2	4		70.8970	66.5011	1	2	-13	5		31.4450	27.3249	1
0	-1	7		34.4270	36.1584	1	2	-11	1		117.1020	118.1027	1
0	-1	9		31.4180	38.6513	1	2	-11	3		111.4570	108.9975	1
							2	-11	5		85.3840	87.7445	1

A2/a	h	k	l	F(obs)	F(calc)	SF*	A2/a	h	k	l	F(obs)	F(calc)	SF*
2	-11	7		70.1720	70.3444	1	3	-6	2		31.0720	31.3128	1
2	-10	8		56.3500	56.3335	1	3	-6	8		36.1570	40.6034	1
2	-10	6		50.4210	50.8148	1	3	-8	2		42.4430	42.7034	1
2	-10	4		61.5100	57.4123	1	3	-8	4		23.7850	19.4486	1
2	-10	2		42.1200	36.9150	1	3	-8	6		25.4590	29.8351	1
2	-9	3		51.8900	49.3718	1	3	-8	8		42.4080	46.8737	1
2	-8	8		86.4780	86.9741	1	3	-9	3		42.2220	41.2598	1
2	-8	6		88.5790	82.9033	1	3	-10	2		24.0260	22.6123	1
2	-8	4		155.9470	162.2900	1	3	-10	4		19.0600	16.7717	1
2	-8	2		150.9750	155.7345	1	3	-11	7		29.0240	29.1104	1
2	-7	1		165.7640	176.1525	1	3	-11	5		73.1000	74.2944	1
2	-7	3		106.7990	108.0777	1	3	-11	3		52.1890	50.0214	1
2	-7	5		84.2390	83.2961	1	3	-11	1		62.8440	64.7903	1
2	-7	7		69.3150	65.4221	1	3	-12	6		31.8660	23.9695	1
2	-7	9		26.9580	30.2019	1	3	-13	3		38.4320	37.3965	1
2	-6	6		37.6900	34.7636	1	3	-14	2		46.0910	44.7112	1
2	-6	4		18.7280	7.0683	1	3	-14	4		36.4620	37.9880	1
2	-6	2		31.1770	28.3573	1	3	-15	3		19.7820	7.7440	1
2	-5	3		118.1500	118.4019	1	3	-15	1		22.2530	22.5068	1
2	-5	5		133.5170	135.1297	1	3	-16	2		24.1480	21.2867	1
2	-5	7		129.8670	133.6768	1	4	-15	1		54.1230	56.9418	1
2	-5	9		80.0840	81.4742	1	4	-15	3		66.0910	63.8585	1
2	-4	10		61.0980	57.0778	1	4	-13	1		43.2410	41.8223	1
2	-4	8		81.3080	83.4803	1	4	-13	3		44.8300	38.9236	1
2	-4	6		94.9610	94.5471	1	4	-13	5		45.7330	44.4113	1
2	-4	4		101.4110	103.7381	1	4	-12	6		59.8340	61.4396	1
2	-4	2		115.4440	117.0342	1	4	-12	4		66.4490	65.4090	1
2	-3	5		41.0190	40.8848	1	4	-12	2		109.4590	105.5384	1
2	-3	7		51.9840	51.7690	1	4	-11	5		20.5880	13.3323	1
2	-3	9		20.8150	19.4829	1	4	-10	6		42.5160	39.9965	1
2	-2	10		60.2770	60.5623	1	4	-10	4		54.0100	51.5087	1
2	-2	8		64.6080	61.6031	1	4	-10	2		22.6260	19.3544	1
2	-2	6		108.9700	110.3304	1	4	-9	1		107.0930	103.7507	1
2	-2	4		132.3850	133.5726	1	4	-9	3		111.8300	112.9586	1
2	-1	3		156.3590	161.5755	1	4	-9	5		88.2760	88.8876	1
2	-1	5		107.8930	106.6629	1	4	-9	7		91.3150	93.3072	1
2	-1	7		74.1350	71.2852	1	4	-8	2		48.4070	46.9767	1
2	-1	9		87.7240	87.8215	1	4	-7	1		72.1070	69.0702	1
2	0	10		32.4610	31.3342	1	4	-7	3		23.9000	27.1862	1
2	0	8		30.5730	21.4021	1	4	-7	7		27.8920	29.0392	1
2	0	4		135.8010	137.1402	1	4	-6	8		70.1130	69.2797	1
3	-1	9		23.0040	26.0600	1	4	-6	6		96.8340	95.5261	1
3	-1	7		23.7410	22.3142	1	4	-6	4		129.2420	133.8589	1
3	-1	3		37.1630	36.6663	1	4	-6	2		116.8350	114.9762	1
3	-2	2		16.6190	11.1509	1	4	-5	1		42.9690	43.4810	1
3	-2	4		22.7990	17.0063	1	4	-5	9		20.8180	16.4532	1
3	-2	6		25.2940	26.7650	1	4	-4	8		26.8270	14.2206	1
3	-2	8		27.6530	13.9988	1	4	-4	6		30.8280	28.8955	1
3	-3	7		19.7730	5.6954	1	4	-4	4		37.7880	37.2816	1
3	-3	5		65.0170	63.8113	1	4	-4	2		13.6270	15.4334	1
3	-3	3		25.0830	19.8952	1	4	-3	5		127.9640	129.7667	1
3	-3	1		69.9610	62.8450	1	4	-3	7		100.4770	99.7185	1
3	-4	2		69.1060	66.6485	1	4	-3	9		93.8940	96.6829	1
3	-4	4		51.1470	50.8740	1	4	-2	8		18.6780	24.6840	1
3	-4	8		27.9350	22.2190	1	4	-2	4		24.3460	23.2574	1
3	-5	3		56.9920	57.4194	1	4	-2	2		66.0340	64.7364	1

A2/a	h	k	l	F(obs)	F(calc)	SF*	A2/a	h	k	l	F(obs)	F(calc)	SF*
4	-1	1		12.1870	14.0674	1	7	-5	1		21.9850	4.4057	1
4	-1	3		27.5570	23.5169	1	7	-6	4		41.6850	38.2156	1
4	-1	5		57.6270	54.9768	1	7	-6	6		22.2050	17.5939	1
4	-1	9		25.6460	20.4852	1	7	-8	2		32.2670	29.2970	1
4	0	8		115.8650	117.5793	1	7	-8	4		47.0400	46.4026	1
4	0	6		155.0160	157.6030	1	7	-8	6		24.4150	26.8987	1
4	0	4		168.6000	175.1586	1	7	-11	3		31.4110	32.8544	1
5	-1	3		34.5810	36.9521	1	7	-11	1		53.3750	52.8404	1
5	-1	1		34.8540	33.5784	1	7	-13	1		17.7520	1.1135	1
5	-2	2		30.1290	33.4232	1	8	-12	2		39.4900	45.9257	1
5	-2	4		27.4650	20.7126	1	8	-10	2		41.9450	37.4791	1
5	-2	6		18.1410	0.7813	1	8	-9	1		65.1010	62.5052	1
5	-3	9		31.8440	27.0000	1	8	-9	3		62.4180	62.9741	1
5	-3	5		39.3850	34.5930	1	8	-8	4		24.2150	22.6115	1
5	-3	3		34.2400	33.9303	1	8	-7	3		23.3900	22.8031	1
5	-3	1		25.3480	26.0158	1	8	-7	5		32.4550	29.5136	1
5	-4	6		47.8840	51.5578	1	8	-6	4		49.7320	48.9128	1
5	-4	8		21.1450	18.6940	1	8	-6	2		77.4000	78.9140	1
5	-5	7		30.1910	29.3003	1	8	-5	5		20.2640	19.2477	1
5	-5	5		18.4430	8.5283	1	8	-4	2		24.6510	22.0070	1
5	-5	1		24.6900	21.8403	1	8	-3	1		94.8180	94.1277	1
5	-6	2		69.8000	69.3606	1	8	-3	3		88.6470	86.7098	1
5	-8	2		52.0970	50.4599	1	8	-3	5		84.6170	82.3990	1
5	-8	4		20.8570	22.8537	1	8	-2	4		28.4340	29.7484	1
5	-9	7		25.7050	27.4020	1	8	-2	2		24.5030	13.7845	1
5	-9	3		17.5540	4.5518	1	8	-1	1		41.7700	46.5784	1
5	-9	1		25.7910	23.3707	1	8	0	6		45.9510	47.4782	1
5	-10	4		21.5180	22.2939	1	8	0	4		99.7010	100.4032	1
5	-11	5		44.9030	41.6593	1	8	0	2		108.5710	108.0341	1
5	-11	3		34.9600	37.0398	1	9	-1	3		18.9840	17.5132	1
5	-12	4		27.8830	31.9487	1	9	-2	4		19.3900	8.9209	1
5	-14	2		35.1720	35.6989	1	9	-3	5		20.2010	19.6054	1
5	-15	1		38.0890	39.6367	1	9	-3	1		48.8210	47.2032	1
6	-14	2		72.0850	69.2088	1	9	-4	2		27.1490	28.9140	1
6	-13	1		23.6280	23.0393	1	9	-5	5		20.0350	10.6798	1
6	-12	4		24.5880	20.0600	1	9	-5	3		24.1570	17.0553	1
6	-12	2		22.8640	20.6174	1	9	-6	4		25.6440	20.2253	1
6	-11	1		69.5310	71.0771	1	9	-8	2		20.2200	0.6552	1
6	-11	3		68.4600	63.7843	1	9	-9	3		25.8610	27.4103	1
6	-11	5		58.3960	56.7889	1	9	-9	1		21.6940	19.1236	1
6	-10	4		41.2350	41.6878	1	9	-10	2		21.8720	16.1320	1
6	-10	2		54.2840	50.5714	1	9	-11	1		32.5430	39.2163	1
6	-9	3		29.1800	23.9039	1	10	-8	2		68.4910	71.5736	1
6	-9	5		20.3030	12.8010	1	10	-7	1		31.7120	34.1977	1
6	-8	6		90.0840	90.5235	1	10	-7	3		26.5160	36.6724	1
6	-8	4		77.0640	75.0628	1	10	-5	3		26.1100	32.9401	1
6	-8	2		83.6650	82.1808	1	10	-5	1		55.8490	50.9232	1
6	0	2		17.8910	10.4942	1	10	-4	2		27.8310	31.2844	1
7	-1	3		29.0050	25.0163	1	10	-2	4		53.5930	52.3779	1
7	-1	1		16.4480	6.0451	1	10	-2	2		39.4570	41.9174	1
7	-2	2		20.6440	12.6706	1	10	-1	1		40.4150	38.2850	1
7	-2	4		20.3010	19.5514	1	10	-1	3		33.9350	37.3026	1
7	-3	7		25.0300	26.8891	1	10	0	4		24.0030	23.3468	1
7	-3	1		41.1780	39.6022	1	10	0	2		52.0350	55.4982	1
7	-4	2		24.4350	23.8898	1	11	-2	0		20.6910	18.3382	1
7	-5	5		22.2070	21.2363	1	11	-3	1		19.1500	8.7289	1

A2/a	h	k	l	F(obs)	F(calc)	SF*	A2/a	h	k	l	F(obs)	F(calc)	SF*
11	-7	1		19.1850	12.0475	1	0	-2	-4		68.8640	66.5022	1
11	-8	0		30.8280	29.3498	1	0	-2	-6		57.8190	57.1259	1
12	-3	1		43.9120	48.9044	1	0	-1	-9		38.5440	38.6507	1
0	-17	-1		20.1560	14.6875	1	0	-1	-7		39.7490	36.1572	1
6	-7	1		46.6930	45.7111	1	0	0	-6		193.4560	199.3429	1
6	-7	3		67.1920	62.7148	1	0	0	-8		132.5560	132.8618	1
6	-7	5		35.5200	35.9979	1	0	0	-10		138.4730	143.2837	1
6	-7	7		59.7360	59.3013	1	1	-2	-10		30.9980	16.7992	1
6	-6	4		19.2430	17.7354	1	1	-1	-5		52.9610	48.0266	1
6	-6	2		27.1430	25.2737	1	1	-2	-8		31.0120	25.7448	1
6	-5	1		121.0610	120.2875	1	1	-2	-6		24.4560	23.3859	1
6	-5	3		132.5380	134.4853	1	1	-2	-4		16.8700	14.6185	1
6	-5	5		78.4940	77.4548	1	1	-6	-6		44.4450	47.0162	1
6	-5	7		57.2270	55.5576	1	1	-6	-8		18.1850	4.5240	1
0	-16	-2		30.4860	28.5217	1	1	-5	-7		36.5460	33.0168	1
0	-16	-4		44.8910	45.7442	1	1	-5	-3		40.0230	35.6888	1
0	-15	-5		52.4570	51.9971	1	1	-4	-4		50.9910	49.7498	1
0	-15	-3		89.9260	92.0346	1	1	-4	-6		51.6290	52.1150	1
0	-15	-1		84.6390	85.7614	1	1	-4	-10		18.3790	17.2567	1
0	-14	-4		20.9960	11.0645	1	1	-3	-9		50.0830	54.1661	1
0	-13	-7		40.2230	42.5405	1	1	-3	-7		16.8880	19.8978	1
0	-13	-5		39.7470	36.8445	1	1	-6	-4		56.0500	56.4325	1
0	-13	-3		65.4890	64.2302	1	1	-6	-2		78.6760	80.1230	1
0	-13	-1		48.7300	48.9501	1	1	-6	0		29.0780	29.4807	1
0	-12	-2		102.9390	103.1316	1	1	-7	-3		21.7750	21.3629	1
0	-12	-4		121.9310	121.7364	1	1	-8	-10		20.4400	14.6937	1
0	-12	-6		106.6640	107.8244	1	1	-8	-6		43.8350	42.1395	1
0	-12	-8		65.4220	65.4119	1	1	-8	-4		65.0570	66.0510	1
0	-11	-1		20.4680	18.1085	1	1	-8	-2		72.9930	69.7859	1
0	-10	-2		63.2800	62.8657	1	1	-8	0		32.5820	32.8593	1
0	-10	-4		28.7410	27.6472	1	1	-9			45.9610	45.6124	1
0	-10	-8		45.0380	46.6587	1	1	-9	-3		18.1300	6.3957	1
0	-9	-9		77.9640	84.0661	1	1	-9	-5		17.0410	13.4542	1
0	-9	-7		90.2350	89.7218	1	1	-9	-7		32.2600	31.7128	1
0	-9	-5		112.0510	115.2488	1	1	-9	-9		18.2740	11.8861	1
0	-9	-3		104.4970	104.1411	1	1	-10	-4		32.7130	35.0270	1
0	-8	-4		20.6510	12.7728	1	1	-10	0		22.8520	24.8509	1
0	-8	-6		33.4390	28.8073	1	1	-11	-1		34.7330	37.1056	1
0	-8	-10		25.2130	19.6236	1	1	-11	-3		49.7690	53.1556	1
0	-7	-7		25.7450	21.8344	1	1	-11	-5		29.9660	34.3709	1
0	-7	-5		81.5600	82.5910	1	1	-11	-7		42.4700	38.9973	1
0	-7	-1		18.5660	15.4027	1	1	-11	-9		59.0030	60.6759	1
0	-6	-4		164.4720	167.5617	1	1	-12	-4		33.9980	33.5572	1
0	-6	-6		118.7870	118.5393	1	1	-13	-1		28.3020	33.3470	1
0	-6	-8		120.7930	124.3215	1	1	-13	-7		34.2340	31.2818	1
0	-6	-10		74.4110	73.3141	1	1	-14	-6		36.2510	39.7593	1
0	-5	-7		21.0780	17.2377	1	1	-14	-4		36.0560	38.4347	1
0	-5	-5		30.4660	31.6194	1	1	-14	-2		46.4690	48.1874	1
0	-5	-3		64.4870	60.1557	1	1	-14	0		41.5770	44.8541	1
0	-4	-6		16.6950	13.6562	1	1	-15	-1		24.8300	26.9890	1
0	-4	-8		31.6410	30.8623	1	1	-15	-3		42.6290	39.4649	1
0	-4	-10		23.5810	28.8590	1	1	-15	-5		35.0620	31.8336	1
0	-3	-11		74.6330	76.6840	1	1	-16	-4		34.8950	34.3248	1
0	-3	-9		103.7310	108.1866	1	1	-16	-2		38.6610	38.0516	1
0	-3	-7		152.8140	157.7928	1	1	-16	0		25.7620	25.8994	1
0	-3	-5		211.6690	216.8840	1	1	-17	-1		34.0270	39.6346	1

A2/a	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*	A2/a	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*
2	-17	-1		59.2720	57.6591	1	2	-2	-6		145.3590	144.0136	1
2	-16	0		29.4440	27.9410	1	2	-2	-8		109.6170	108.3643	1
2	-16	-4		36.4750	29.0575	1	2	-2	-10		84.2700	84.7565	1
2	-14	0		84.9280	84.3548	1	2	-2	-12		33.6740	35.3547	1
2	-14	-2		76.4150	76.9111	1	2	-1	-11		59.0230	59.8565	1
2	-14	-4		92.3760	91.1092	1	2	-1	-9		63.1820	60.7557	1
2	-14	-6		48.9590	47.9688	1	2	-1	-7		118.6770	117.5750	1
2	-13	-7		40.0950	38.5370	1	2	-1	-5		93.5660	88.7904	1
2	-13	-3		32.4970	30.4571	1	2	0	-6		100.0550	97.4209	1
2	-13	-1		34.9510	38.4801	1	2	0	-8		79.6820	76.9283	1
2	-12	0		21.3180	17.3452	1	3	-1	-11		34.0620	32.5535	1
2	-12	-2		44.0560	45.6454	1	3	-2	-6		34.9590	35.4613	1
2	-12	-4		22.7240	19.7650	1	3	-3	-3		18.0620	17.9713	1
2	-12	-6		19.8460	0.4120	1	3	-3	-5		99.9350	100.7070	1
2	-11	-9		68.0680	72.0848	1	3	-3	-7		32.4880	29.7773	1
2	-11	-7		88.9040	87.8555	1	3	-4	-10		24.7000	19.2244	1
2	-11	-5		99.1250	99.4927	1	3	-4	-8		37.4460	38.8439	1
2	-11	-3		99.2820	98.8466	1	3	-4	-6		19.7100	19.2514	1
2	-11	-1		100.5650	103.2853	1	3	-4	-4		32.5990	32.1824	1
2	-10	0		60.7420	60.6392	1	3	-4	-2		42.7000	39.2326	1
2	-10	-2		97.6580	97.3130	1	3	-4	0		65.4660	63.7274	1
2	-10	-4		57.8810	56.9416	1	3	-5	-1		16.0040	12.0416	1
2	-10	-6		42.1440	43.2824	1	3	-5	-3		49.8950	47.4409	1
2	-10	-8		36.9640	39.1043	1	3	-5	-7		31.3520	29.1935	1
2	-10	-10		36.2470	35.0564	1	3	-6	-10		18.0850	22.5339	1
2	-9	-7		40.8700	40.5750	1	3	-6	-8		25.0780	28.0404	1
2	-9	-3		15.5430	6.6504	1	3	-6	-4		15.1240	17.8615	1
2	-9	-1		17.0530	14.4960	1	3	-6	-2		93.7070	95.1612	1
2	-8	0		153.2760	153.8931	1	3	-6	0		48.1380	46.5772	1
2	-8	-2		180.0990	184.9100	1	3	-7	-3		15.6360	7.0315	1
2	-8	-4		116.0590	116.9401	1	3	-8	-10		35.9180	37.6183	1
2	-8	-6		132.7900	138.0353	1	3	-8	-8		28.4030	32.2563	1
2	-8	-8		117.8110	117.3881	1	3	-8	-4		32.5630	36.3689	1
2	-8	-10		61.2740	60.9975	1	3	-8	-2		77.1250	80.2562	1
2	-7	-11		42.5620	41.7492	1	3	-8	0		69.4270	69.4972	1
2	-7	-9		81.7840	82.0510	1	3	-9	-1		15.2240	6.5178	1
2	-7	-7		78.5040	77.8790	1	3	-9	-3		19.5130	25.6949	1
2	-7	-5		119.8700	121.7249	1	3	-9	-5		17.9510	14.2494	1
2	-7	-3		77.3620	74.3545	1	3	-9	-7		23.9900	25.5674	1
2	-7	-1		70.7830	66.5285	1	3	-10	-8		19.4560	22.4013	1
2	-6	0		38.7900	36.9832	1	3	-10	-2		15.8500	13.0414	1
2	-6	-4		46.8650	45.8763	1	3	-10	0		30.4240	27.0717	1
2	-6	-10		24.8190	18.3178	1	3	-11	-1		41.6500	44.7185	1
2	-5	-11		84.6360	88.3499	1	3	-11	-3		28.1370	31.9357	1
2	-5	-9		95.7280	95.0494	1	3	-11	-5		86.1860	87.4958	1
2	-5	-7		86.6410	84.5757	1	3	-11	-7		48.5880	49.8854	1
2	-5	-5		162.1890	166.4728	1	3	-12	-4		20.6040	16.2352	1
2	-5	-3		230.5880	239.0708	1	3	-12	0		31.9540	31.2859	1
2	-4	-6		92.5260	91.3351	1	3	-13	-3		18.1560	12.5785	1
2	-4	-8		69.5130	70.5266	1	3	-13	-7		25.4270	21.9594	1
2	-4	-10		66.0440	65.2386	1	3	-14	-6		27.1240	29.3081	1
2	-4	-12		61.8100	60.9700	1	3	-14	-4		37.5390	40.2812	1
2	-3	-11		21.9050	23.1731	1	3	-14	-2		53.8440	57.2511	1
2	-3	-9		17.4300	20.7818	1	3	-14	0		42.0840	43.4711	1
2	-3	-5		55.6810	51.7186	1	3	-15	-1		34.3450	35.6302	1
2	-2	-4		179.3100	176.9731	1	3	-15	-3		19.0210	23.6889	1

A2/a	h	k	l	F(obs)	F(calc)	SF*	A2/a	h	k	l	F(obs)	F(calc)	SF*
3	-16	-4		24.1560	15.9213	1	4	-3	-11		99.1430	99.4893	1
3	-16	-2		35.0620	34.2731	1	4	-3	-9		122.9770	122.2272	1
3	-16	0		25.0810	25.0486	1	4	-3	-7		153.2310	150.5802	1
4	-16	0		41.7390	39.6270	1	4	-3	-3		190.3540	189.4636	1
4	-16	-2		37.6200	38.9921	1	4	-2	0		57.8500	52.4818	1
4	-16	-4		41.0190	38.3960	1	4	-2	-2		35.8720	32.2631	1
4	-15	-5		77.6520	76.9392	1	4	-2	-4		15.0730	9.1460	1
4	-15	-3		62.5740	61.9078	1	4	-2	-6		25.7440	26.1484	1
4	-15	-1		80.7060	80.6658	1	4	-2	-8		39.1310	37.9469	1
4	-14	-4		33.7720	31.1549	1	4	-2	-10		31.9410	34.6179	1
4	-13	-7		47.0740	47.8284	1	4	-1	-11		29.5610	33.6748	1
4	-13	-5		50.3920	47.6349	1	4	-1	-7		48.1230	47.3552	1
4	-13	-3		33.2630	39.8774	1	4	-1	-5		63.3010	63.8826	1
4	-13	-1		62.5730	63.3049	1	4	-1	-3		20.2370	16.1669	1
4	-12	0		115.9800	115.0521	1	4	0	-6		179.1720	179.1909	1
4	-12	-2		96.9620	98.1910	1	4	0	-8		147.7080	144.6306	1
4	-12	-4		76.9000	78.9229	1	4	0	-10		99.5560	96.0018	1
4	-12	-6		65.3400	66.8843	1	4	0	-12		73.7070	71.9318	1
4	-12	-8		80.1420	82.9666	1	5	-1	-1		28.3640	26.8933	1
4	-11	-7		17.9860	3.5937	1	5	-1	-3		37.4620	37.2985	1
4	-10	0		30.6010	31.8970	1	5	-1	-5		22.0500	23.4450	1
4	-10	-2		40.4540	41.0984	1	5	-1	-7		37.0060	36.4869	1
4	-10	-4		49.4980	50.2021	1	5	-2	-12		22.0910	14.3877	1
4	-10	-6		57.1180	58.4796	1	5	-2	-10		25.9820	21.4989	1
4	-10	-8		21.0190	19.2797	1	5	-2	-8		20.0050	12.7463	1
4	-10	-10		19.7830	15.3461	1	5	-2	-4		23.0650	23.2956	1
4	-9	-11		48.2270	43.4548	1	5	-2	-2		40.1490	36.8646	1
4	-9	-9		76.6280	74.3090	1	5	-2	0		33.3920	32.2844	1
4	-9	-7		78.3650	81.6278	1	5	-3	-1		79.8250	79.0468	1
4	-9	-5		117.8410	118.0641	1	5	-3	-3		73.4520	75.0919	1
4	-9	-3		142.6390	144.5677	1	5	-3	-5		25.7100	26.1884	1
4	-9	-1		83.0620	82.3363	1	5	-3	-7		35.2710	38.6015	1
4	-8	-2		24.2290	23.0023	1	5	-3	-9		18.6330	7.3555	1
4	-8	-4		54.3360	56.7615	1	5	-4	-8		18.8380	20.0005	1
4	-8	-6		19.3920	2.1519	1	5	-4	-4		81.0630	81.7613	1
4	-8	-8		26.9820	17.6283	1	5	-5	-1		22.6750	23.4865	1
4	-7	-9		57.2120	59.0014	1	5	-5	-3		17.4770	13.0005	1
4	-7	-5		15.9520	7.3812	1	5	-5	-5		16.6920	21.3726	1
4	-7	-3		38.3710	39.0776	1	5	-5	-7		32.6730	28.6488	1
4	-7	-1		20.1600	19.9527	1	5	-5	-11		19.2240	2.4877	1
4	-6	0		172.9530	175.7888	1	5	-6	-10		36.8360	37.4820	1
4	-6	-2		159.7810	159.8100	1	5	-6	-8		39.9050	44.6133	1
4	-6	-4		117.4270	117.3344	1	5	-6	-6		30.0680	30.9952	1
4	-6	-6		139.2530	141.6119	1	5	-6	-4		23.1610	26.8371	1
4	-6	-8		91.5930	90.8736	1	5	-6	0		61.9500	61.8235	1
4	-6	-10		79.7410	78.4582	1	5	-8	-10		25.6970	23.8992	1
4	-6	-12		71.7260	72.9350	1	5	-8	-8		32.8320	35.4883	1
4	-5	-11		22.6250	15.1653	1	5	-8	-6		18.2340	25.1850	1
4	-5	-7		24.3830	17.0038	1	5	-8	0		45.6300	46.2423	1
4	-5	-3		19.1190	18.4121	1	5	-9	-1		18.4320	16.1658	1
4	-5	-1		75.0770	73.4983	1	5	-9	-3		38.0760	40.3264	1
4	-4	-2		36.1610	35.1959	1	5	-9	-5		37.8130	39.9417	1
4	-4	-4		51.4530	52.6295	1	5	-9	-11		26.0840	16.0511	1
4	-4	-6		45.1270	43.5397	1	5	-10	-4		27.4200	31.0755	1
4	-4	-8		21.7400	15.6584	1	5	-10	-2		20.0750	6.4688	1
4	-4	-12		30.2720	20.9376	1	5	-11	-1		54.2160	55.5463	1

A2/a	h	k	l	F(obs)	F(calc)	SF*	A2/a	h	k	l	F(obs)	F(calc)	SF*
5	-11	-3		54.5290	56.1793	1	6	-4	0		87.6720	85.7383	1
5	-11	-5		26.1600	29.8881	1	6	-4	-2		72.0420	69.6475	1
5	-11	-7		29.3810	33.1059	1	6	-4	-4		82.7530	81.3768	1
5	-12	-6		26.0470	27.0862	1	6	-4	-6		91.1690	91.8112	1
5	-12	-2		40.9550	43.2005	1	6	-4	-8		71.8900	71.8400	1
5	-13	-3		31.8070	32.9083	1	6	-4	-10		53.8230	49.3429	1
5	-13	-5		22.8490	28.3648	1	6	-4	-12		36.8110	33.4638	1
5	-14	-6		23.9760	19.8733	1	6	-3	-9		24.1170	22.8905	1
5	-14	0		28.7060	32.0748	1	6	-3	-7		49.2820	50.3234	1
5	-15	-1		21.4370	26.8335	1	6	-3	-5		34.4840	32.5858	1
5	-16	-2		25.2430	16.1023	1	6	-3	-3		29.3110	27.8970	1
6	-15	-3		24.9870	22.2993	1	6	-3	-1		15.0100	21.6067	1
6	-14	0		37.1640	36.4351	1	6	-2	0		94.0980	91.9987	1
6	-14	-2		49.7100	50.4023	1	6	-2	-2		169.2440	171.9146	1
6	-14	-4		45.0010	46.5384	1	6	-2	-4		111.5310	111.9926	1
6	-14	-6		53.2620	53.8771	1	6	-2	-6		59.8260	59.1157	1
6	-13	-5		29.7300	27.2015	1	6	-2	-8		76.1930	75.2398	1
6	-13	-3		17.9380	10.7417	1	6	-2	-10		61.1920	59.6939	1
6	-12	0		20.5520	12.4000	1	6	-2	-12		65.2160	65.1936	1
6	-13	-1		25.6370	22.5164	1	6	-1	-11		59.9670	57.0419	1
6	-12	-6		21.4130	24.3474	1	6	-1	-9		58.4050	55.5200	1
6	-11	-9		57.3580	55.2213	1	6	-1	-7		66.9500	65.7023	1
6	-11	-7		64.9370	61.4833	1	6	-1	-5		119.1770	117.3919	1
6	-11	-5		67.5410	69.7560	1	6	-1	-3		58.7090	54.6989	1
6	-11	-3		87.1540	87.4754	1	6	-1	-1		95.9570	90.6319	1
6	-11	-1		87.2240	89.0331	1	6	0	0		105.1400	106.5156	1
6	-10	0		50.9820	48.6928	1	6	0	-2		71.4980	71.4789	1
6	-10	-4		41.3120	39.1535	1	6	-4	8		36.4920	35.9842	1
6	-10	-6		53.2380	55.8591	1	6	-4	6		56.5710	53.0691	1
6	-10	-8		37.0690	37.3170	1	6	-4	4		75.2500	75.7662	1
6	-10	-10		31.0530	30.7054	1	6	-4	2		89.6130	87.1784	1
6	-9	-7		20.6760	23.2615	1	6	-3	1		40.9930	40.4115	1
6	-9	-5		20.4090	14.5360	1	6	-3	3		58.5090	58.1944	1
6	-9	-3		20.5700	7.1292	1	6	-3	5		26.6300	22.6182	1
6	-9	-1		27.7280	24.2556	1	6	-2	8		72.0010	76.5110	1
6	-8	0		134.4920	135.4143	1	6	-2	6		66.5670	59.4983	1
6	-8	-2		103.5800	105.3086	1	6	-2	4		69.9690	69.7967	1
6	-8	-4		118.0570	119.9593	1	6	-2	2		83.7820	81.4580	1
6	-8	-6		101.7240	103.6772	1	6	-1	1		107.9630	107.8354	1
6	-8	-8		62.5520	61.5453	1	6	-1	3		56.2100	54.7229	1
6	-8	-10		81.1720	84.3382	1	6	-1	5		82.4310	78.7399	1
6	-7	-11		48.3970	44.2096	1	6	-1	7		47.7830	47.0889	1
6	-7	-9		53.9460	51.0202	1	6	0	6		55.0890	57.6012	1
6	-7	-7		49.1830	47.9545	1	6	0	4		26.4310	15.8265	1
6	-7	-5		34.9690	37.0182	1	6	0	-4		76.6090	78.2363	1
6	-7	-3		114.6230	117.8135	1	6	0	-6		34.8500	36.6765	1
6	-7	-1		91.0510	91.3891	1	6	0	-10		42.5500	46.3693	1
6	-6	-2		29.7710	29.1326	1	6	0	-12		27.2990	28.6525	1
6	-6	-8		27.8110	21.3532	1	7	-1	-1		40.9850	44.3497	1
6	-6	-10		23.3510	10.8713	1	7	-1	-5		21.6290	20.2515	1
6	-5	-11		48.7570	43.8317	1	7	-1	-11		21.2060	24.3106	1
6	-5	-9		90.6950	89.0358	1	7	-2	-6		45.4620	44.7650	1
6	-5	-7		128.4710	129.9507	1	7	-3	-1		21.1200	22.2810	1
6	-5	-5		112.0010	114.2933	1	7	-3	-3		55.8310	56.3103	1
6	-5	-3		115.9530	117.0577	1	7	-3	-7		16.6660	1.0127	1
6	-5	-1		103.2250	101.7005	1	7	-3	-9		44.9560	41.8476	1



A2/a	h	k	l	F(obs)	F(calc)	SF*	A2/a	h	k	l	F(obs)	F(calc)	SF*
7	-4	-8		20.2150	15.9687	1	8	-6	0		82.7160	81.6576	1
7	-4	-4		33.5630	32.9203	1	8	-6	-2		66.5350	67.9102	1
7	-4	-2		23.4770	18.0501	1	8	-6	-4		99.5850	99.3939	1
7	-4	0		41.8930	42.8359	1	8	-6	-6		66.2580	67.0293	1
7	-5	-1		34.0510	34.1733	1	8	-6	-8		57.8160	58.5800	1
7	-5	-3		17.8040	19.0060	1	8	-6	-10		61.8410	62.8230	1
7	-5	-11		23.0700	19.0746	1	8	-5	-5		40.7040	42.8528	1
7	-6	-6		54.4190	56.3830	1	8	-5	-3		32.1250	32.5350	1
7	-6	-4		24.3730	25.9923	1	8	-4	0		28.9900	30.3363	1
7	-6	0		18.8740	10.8651	1	8	-4	-6		23.2280	11.8826	1
7	-7	-3		16.2290	9.8874	1	8	-4	-8		27.8910	25.1079	1
7	-8	-8		24.7550	22.5230	1	8	-4	-10		26.6490	27.1112	1
7	-8	-6		53.4300	50.2311	1	8	-4	-12		19.9210	12.2093	1
7	-8	-4		34.9270	37.0665	1	8	-3	-11		58.9750	58.3616	1
7	-8	-2		24.9200	18.8971	1	8	-3	-9		70.7520	69.8355	1
7	-9	-1		32.7110	32.3829	1	8	-3	-7		85.0930	86.2036	1
7	-10	-10		19.4740	21.5399	1	8	-3	-5		128.2420	128.0108	1
7	-10	-2		26.9000	27.0296	1	8	-3	-3		126.2790	128.0336	1
7	-10	0		38.1600	37.2461	1	8	-3	-1		97.8110	94.3503	1
7	-11	-1		46.5590	43.5019	1	8	-2	0		17.8440	16.0518	1
7	-11	-3		60.7120	60.8149	1	8	-2	-2		26.1680	24.6100	1
7	-11	-5		26.0710	18.5550	1	8	-2	-6		29.6540	28.7554	1
7	-11	-9		44.7550	50.1763	1	8	-2	-12		22.2520	22.6757	1
7	-13	-1		24.0110	21.0750	1	8	-1	-9		38.9510	38.5217	1
7	-13	-5		21.5570	16.8840	1	8	-1	-5		32.2720	31.2448	1
7	-14	-6		41.4380	40.0685	1	8	-1	-3		22.6270	24.5689	1
7	-14	-4		31.5810	31.5469	1	8	0	0		141.3230	143.8633	1
7	-14	-2		35.4220	28.0436	1	8	0	-2		151.6730	153.9396	1
7	-14	0		36.2180	35.8165	1	8	0	-4		79.6760	76.7739	1
8	-14	-4		22.3890	19.0921	1	8	0	-6		116.8700	117.2645	1
8	-13	-5		47.1310	45.3829	1	8	0	-8		124.9530	122.0362	1
8	-13	-3		31.2600	38.4472	1	8	0	-10		84.9240	84.2594	1
8	-13	-1		31.9320	28.6962	1	8	0	-12		72.3790	73.5294	1
8	-12	0		43.3830	41.0463	1	9	-1	-3		16.6890	12.2472	1
8	-12	-2		66.3970	65.7050	1	9	-1	-7		26.6350	28.6866	1
8	-12	-4		71.6440	71.0460	1	9	-1	-9		19.7660	20.5843	1
8	-12	-6		61.7820	63.2365	1	9	-2	-12		21.8630	18.8144	1
8	-12	-8		33.8800	40.5797	1	9	-2	-8		20.8200	18.3434	1
8	-11	-3		21.3450	1.7333	1	9	-2	-4		27.0440	23.2744	1
8	-10	0		36.9270	40.2336	1	9	-2	-2		40.5030	40.3608	1
8	-10	-2		23.6950	22.6795	1	9	-3	-1		26.9940	20.6164	1
8	-10	-4		19.3730	24.3146	1	9	-3	-5		42.9170	39.5674	1
8	-10	-8		38.4450	34.8085	1	9	-3	-7		27.3490	25.0107	1
8	-9	-9		52.6170	53.0731	1	9	-3	-9		27.6490	28.2048	1
8	-9	-7		69.7970	71.8362	1	9	-4	-8		38.2860	34.3920	1
8	-9	-5		37.3710	41.2408	1	9	-5	-3		18.1790	5.5253	1
8	-9	-3		51.0510	51.9520	1	9	-5	-5		32.1580	30.2873	1
8	-9	-1		84.5790	87.3759	1	9	-5	-9		19.2390	4.0425	1
8	-8	0		26.0700	23.0197	1	9	-5	-11		26.6890	19.2397	1
8	-8	-2		40.5930	36.2749	1	9	-6	-6		20.6050	15.3684	1
8	-8	-6		22.0120	21.0698	1	9	-6	-4		43.1130	40.2551	1
8	-8	-8		23.2750	21.1075	1	9	-6	-2		55.1000	54.3100	1
8	-7	-7		31.3580	31.0073	1	9	-7	-7		22.9220	9.8669	1
8	-7	-5		31.0040	25.6532	1	9	-8	-8		17.6170	7.0288	1
8	-7	-3		30.4750	28.3490	1	9	-8	-4		19.3490	24.2662	1
8	-7	-1		22.6460	21.0270	1	9	-8	-2		18.6140	26.5163	1

A2/a	h	k	l	F(obs)	F(calc)	SF*	A2/a	h	k	l	F(obs)	F(calc)	SF*
9	-9	-1		20.3590	13.7119	1	11	-2	-4		22.9600	21.1061	1
9	-9	-3		23.9210	15.0948	1	11	-2	-8		20.0430	12.8724	1
9	-10	-8		26.1290	27.0436	1	11	-2	-10		22.0670	27.0629	1
9	-9	-7		38.6630	29.3335	1	11	-3	-1		23.5390	16.1177	1
9	-11	-5		18.4400	25.7495	1	11	-3	-7		38.7020	34.6114	1
9	-12	-6		25.8860	24.3096	1	11	-4	-2		29.9220	25.2824	1
9	-12	-4		25.5820	21.6655	1	11	-4	0		21.1210	14.9176	1
9	-12	0		25.0180	28.6430	1	11	-5	-9		19.9630	0.0844	1
10	-11	-7		43.8200	45.4834	1	11	-5	-7		18.3730	15.0155	1
10	-11	-1		35.3280	37.9217	1	11	-5	-1		22.2290	20.6243	1
10	-11	-3		36.1580	38.9700	1	11	-6	-10		29.0030	29.2216	1
10	-11	-5		46.2230	49.9228	1	11	-6	-2		22.2030	15.8590	1
10	-10	-2		31.4940	35.6086	1	11	-7	-5		18.3540	18.2788	1
10	-10	-4		22.1790	25.6278	1	11	-7	-7		21.7680	14.7177	1
10	-9	-9		20.0730	4.8410	1	11	-8	-2		27.8830	19.3375	1
10	-8	0		44.4340	44.6371	1	11	-9	-1		19.0310	12.3025	1
10	-8	-2		58.0540	58.7203	1	11	-9	-5		23.9810	16.3354	1
10	-8	-4		69.6310	70.9428	1	11	-10	-6		30.1840	23.2619	1
10	-8	-6		54.2790	52.6457	1	11	-10	-4		41.0110	37.3934	1
10	-8	-8		67.4930	69.1020	1	12	-8	-4		24.8390	24.9872	1
10	-7	-7		52.5780	56.2211	1	12	-8	-6		28.9460	19.1055	1
10	-7	-5		51.9620	53.1628	1	12	-6	-2		37.7630	42.6220	1
10	-7	-1		36.7290	35.8458	1	12	-6	-4		26.1500	28.4648	1
10	-6	-8		19.3670	9.7215	1	12	-6	-6		25.7760	28.6317	1
10	-6	-10		21.7190	1.6193	1	12	-6	-8		38.4660	39.8139	1
10	-5	-11		59.0600	62.8427	1	12	-5	-9		26.9390	22.5925	1
10	-5	-9		44.3400	44.9503	1	12	-5	-7		21.3970	18.0531	1
10	-5	-7		45.8310	45.3937	1	12	-5	-5		26.2570	8.6137	1
10	-5	-5		58.0910	59.0839	1	12	-4	-4		23.3640	17.8221	1
10	-5	-3		71.4780	71.4730	1	12	-4	-8		19.7850	2.8353	1
10	-5	-1		86.0380	86.9142	1	12	-3	-9		52.4880	52.1828	1
10	-4	0		40.9760	43.2773	1	12	-3	-7		52.8930	53.8381	1
10	-4	-2		49.7800	51.4440	1	12	-3	-5		29.9500	36.2465	1
10	-4	-4		47.2430	44.5866	1	12	-3	-3		37.1860	44.5571	1
10	-4	-6		27.4430	27.3810	1	12	-3	-1		47.9960	53.9705	1
10	-4	-8		31.9820	29.7709	1	12	-2	-2		22.1200	8.7128	1
10	-4	-10		30.7620	36.6932	1	12	-1	-3		19.3760	24.4856	1
10	-3	-11		30.7390	21.8634	1	12	0	0		52.5840	54.3716	1
10	-3	-5		20.9680	16.6946	1	12	0	-2		45.4490	48.8598	1
10	-3	-3		27.9200	25.8822	1	12	0	-4		81.4170	84.9030	1
10	-3	-1		39.0240	36.9886	1	12	0	-6		65.4640	69.5082	1
10	-2	-2		30.3890	29.6333	1	12	0	-8		24.1280	28.9030	1
10	-2	0		52.1940	50.5871	1	12	0	-10		42.7210	45.3654	1
10	-2	-6		75.2830	76.5822	1	13	-1	-5		21.4420	11.7826	1
10	-2	-8		43.1100	45.5481	1	13	-3	-3		36.1850	38.0205	1
10	-2	-4		39.8650	40.3027	1	13	-2	-6		32.8750	28.4162	1
10	-2	-10		34.4960	28.6306	1	13	-2	-8		22.6160	16.0274	1
10	-1	-9		37.2200	43.2245	1	13	-4	-2		21.5810	6.2024	1
10	-1	-5		34.9450	27.7312	1	13	-5	-3		22.3450	17.7459	1
10	-1	-3		59.8060	60.8347	1	13	-5	-7		19.8230	16.0007	1
10	-1	-1		32.5010	28.0431	1	13	-6	-6		31.9770	29.1612	1
10	0	-8		49.7530	49.2064	1	13	-6	-4		19.3840	3.7959	1
10	0	-6		35.1510	31.4853	1	0	-5	-1		28.1520	28.2855	2
10	0	-4		47.1230	41.9252	1	0	-5	1		28.5740	28.2856	2
10	0	-2		22.6790	14.8383	1	0	-4	2		46.5340	45.0687	2
11	-1	-5		34.2520	30.2870	1	0	-4	0		63.5430	64.5087	2

A2/a	h	k	l	F(obs)	F(calc)	SF*
0	-4	-2		45.6710	45.0680	2
0	-2	2		19.7040	15.0646	2
0	-2	0		23.7380	21.4050	2
0	-2	-2		19.4620	15.0645	2
0	-1	-3		94.2770	94.4917	2
0	-1	-1		60.2380	58.4419	2
0	-1			59.2310	58.4422	2
0	-1	3		94.5740	94.4918	2
1	-1	3		10.5910	9.0366	2
1	-1	1		22.7280	17.2186	2
1	-1	-3		106.2810	105.7312	2
1	-2	-2		29.1420	27.5874	2
1	-2	0		7.6390	4.7152	2
1	-2	2		73.9520	73.8454	2
1	-3	-1		11.2940	7.5928	2
1	-4	-2		28.0430	28.6935	2
1	-4	0		109.7420	110.2337	2
1	-5	-1		57.3720	56.9556	2
2	-4	0		121.1930	126.4817	2
2	-4	-2		144.0050	154.5468	2
2	-3	-3		73.7450	73.6409	2
2	-3	-1		69.3560	67.3767	2
2	-3	1		46.9800	46.0052	2
2	-2	-2		45.9500	52.3549	2
2	-1	-3		129.7970	137.1564	2
2	-1	1		54.3610	58.1678	2
2	0	2		98.5770	101.3978	2
2	0	0		58.1150	55.3761	2
2	0	-2		88.0680	85.6970	2
3	-1	1		50.6830	47.2810	2
3	-1	-1		98.9210	97.5266	2
3	-1	-3		20.8980	18.2462	2
3	-2	-2		58.8560	54.0558	2
3	-2	0		21.8070	21.9670	2
3	-3	-1		14.9550	13.7924	2
4	-1	-1		78.1430	78.4047	2
0	-6	2		211.3760	220.6180	1
4	-3	1		218.1890	233.6590	1
4	-3	3		154.5340	163.3434	1
0	-9	-1		165.8130	177.3750	1
0	-6	-2		209.6420	220.6179	1
0	0	-4		224.3290	227.2077	1
2	-5	-1		231.8920	239.6473	1
2	-4	-4		145.8050	144.0496	1
4	-3	-1		266.8811	279.6313	1
4	-3	-5		158.5800	161.3908	1

P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*
0	-16	4		21.2842	22.2330	1	0	-3	3		142.9948	142.8745	1
0	-16	2		14.5994	14.7540	1	0	-3	5		102.1097	100.7987	1
0	-16	0		22.5450	22.4747	1	0	-3	7		74.8229	73.0757	1
0	-15	1		39.2647	39.5706	1	0	-3	9		51.9392	49.3260	1
0	-15	3		44.5311	42.5144	1	0	-3	11		34.1027	34.2140	1
0	-15	5		26.8569	23.5837	1	0	-2	11		9.3102	3.7587	1
0	-14	4		9.5807	3.7120	1	0	-2	6		26.9401	25.6969	1
0	-14	0		18.6210	18.0097	1	0	-2	4		33.0630	30.8063	1
0	-13	1		23.1455	23.4702	1	0	-1	7		15.9652	16.1864	1
0	-13	3		29.6440	29.9766	1	0	-1	9		14.4568	16.9042	1
0	-13	5		18.8972	18.2076	1	1	-1	7		22.8441	22.8765	1
0	-13	7		20.0869	21.0832	1	1	-1	5		15.6061	16.1295	1
0	-12	8		29.6188	30.1816	1	1	-2	4		12.3368	13.6132	1
0	-12	6		50.2037	49.2608	1	1	-2	7		7.8477	6.5818	1
0	-12	4		58.9558	55.6743	1	1	-3	11		10.2803	7.4869	1
0	-12	2		47.8812	47.4199	1	1	-3	7		14.2338	13.8570	1
0	-12	0		48.6554	46.5759	1	1	-3	5		7.7873	8.6480	1
0	-11	1		9.4742	7.5047	1	1	-3	3		39.0866	35.8111	1
0	-10	9		9.6563	0.4457	1	1	-4	2		15.5263	15.2997	1
0	-10	8		21.2442	21.0616	1	1	-4	4		25.8962	26.6191	1
0	-10	4		13.1521	13.1322	1	1	-4	7		8.5686	0.9539	1
0	-10	2		29.3264	29.6798	1	1	-4	8		7.9178	1.1200	1
0	-10	0		28.9927	27.4248	1	1	-4	10		20.3368	20.5833	1
0	-9	1		79.9688	82.0350	1	1	-5	9		12.7246	11.6519	1
0	-9	3		50.4193	47.7668	1	1	-5	7		7.6183	5.1437	1
0	-9	5		54.0915	53.1641	1	1	-5	5		15.4099	14.7121	1
0	-9	7		43.2499	41.3438	1	1	-5	3		10.5632	6.9553	1
0	-9	-9		39.4937	38.4260	1	1	-5	1		7.2800	4.1285	1
0	-8	6		10.7359	12.4223	1	1	-6	2		11.0029	11.4463	1
0	-8	2		6.9772	4.9899	1	1	-6	4		27.2332	26.7912	1
0	-8	1		7.5320	1.7702	1	1	-6	6		24.8320	23.1559	1
0	-8	0		40.8737	40.0691	1	1	-6	7		7.5930	8.2729	1
0	-7	1		6.8523	6.9984	1	1	-6	8		12.2177	8.4206	1
0	-7	3		8.2893	4.8835	1	1	-8	2		7.1316	6.3929	1
0	-7	5		40.0657	38.2320	1	1	-8	4		24.9962	24.4457	1
0	-7	6		10.5004	1.4984	1	1	-8	6		25.5175	25.5316	1
0	-6	11		9.5414	3.9940	1	1	-8	8		16.9422	15.7941	1
0	-6	10		33.6653	33.5608	1	1	-8	10		9.8524	6.9515	1
0	-6	8		58.4736	56.2983	1	1	-9	7		8.3906	3.7668	1
0	-6	6		56.1914	54.0568	1	1	-9	5		8.2479	8.6694	1
0	-6	4		76.8993	77.9039	1	1	-9	3		14.3434	12.7346	1
0	-6	2		103.9680	103.4145	1	1	-9	1		15.0071	15.0875	1
0	-6	0		75.5870	73.5600	1	1	-10	6		13.1453	9.0159	1
0	-5	3		30.2889	28.4695	1	1	-10	8		8.3734	7.8533	1
0	-5	5		12.4669	14.8362	1	1	-11	7		21.0793	19.0429	1
0	-5	7		10.0869	8.4234	1	1	-11	3		31.9290	31.0914	1
0	-5	11		9.1971	9.3813	1	1	-11	1		45.9235	43.6372	1
0	-4	10		12.7671	12.8923	1	1	-12	2		23.0428	20.3338	1
0	-4	8		16.4786	14.2533	1	1	-13	5		8.3262	5.6079	1
0	-4	6		8.9692	5.9370	1	1	-13	3		8.9141	8.6077	1
0	-4	4		8.2810	6.2006	1	1	-13	1		13.5734	11.7685	1
							1	-14	2		14.6276	12.8010	1
							1	-14	4		22.6214	19.9344	1
							1	-14	6		17.3940	17.0639	1
							1	-15	3		12.8811	8.4374	1

P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*
1	-14	6		17.3940	17.0639	1	2	0	10		15.0474	13.5842	1
1	-15	3		12.8811	8.4374	1	2	0	8		14.1676	9.6523	1
1	-15	5		17.9613	14.7427	1	2	0	4		64.5769	64.1515	1
1	-17	1		14.4164	7.3496	1	3	-1	9		10.6627	13.8097	1
2	-16	3		11.0083	7.5944	1	3	-1	7		11.0046	10.9073	1
2	-16	2		20.1744	17.6837	1	3	-1	3		17.2471	16.5831	1
2	-16	1		9.1805	6.5808	1	3	-2	2		7.7002	5.2573	1
2	-15	1		16.6112	13.0329	1	3	-2	4		10.5660	8.9402	1
2	-14	4		20.1690	20.2850	1	3	-2	6		11.7247	12.5470	1
2	-14	2		29.6246	28.3914	1	3	-2	8		12.8115	5.6179	1
2	-13	1		14.2050	9.3352	1	3	-3	10		8.5348	4.1833	1
2	-13	3		20.0768	19.2806	1	3	-3	7		9.1598	2.1222	1
2	-13	5		14.5757	13.7110	1	3	-3	5		30.2334	29.4937	1
2	-11	1		54.8450	55.0039	1	3	-3	3		11.6270	10.3998	1
2	-11	3		52.0797	50.1461	1	3	-3	1		32.6343	29.1641	1
2	-11	5		39.7562	39.4216	1	3	-4	2		32.2200	32.0162	1
2	-11	7		32.6177	32.0463	1	3	-4	4		23.7620	24.5311	1
2	-10	8		26.1635	26.3954	1	3	-4	8		12.9451	9.9246	1
2	-10	6		23.3994	23.2647	1	3	-5	3		26.4944	26.4431	1
2	-10	4		28.5620	26.2733	1	3	-6	2		14.4097	14.6168	1
2	-10	2		19.5352	17.4742	1	3	-6	8		16.7687	18.4519	1
2	-9	3		24.0830	22.0070	1	3	-8	2		19.6931	19.4537	1
2	-8	8		40.2613	39.0088	1	3	-8	4		11.0210	8.2874	1
2	-8	6		41.2925	38.7904	1	3	-8	6		11.8014	13.8429	1
2	-8	4		73.7731	75.4618	1	3	-8	8		19.6743	21.0851	1
2	-8	2		71.5880	72.7864	1	3	-9	3		19.5854	18.8400	1
2	-7	1		79.4995	82.6127	1	3	-10	2		11.1351	11.2125	1
2	-7	3		50.0587	50.7633	1	3	-10	4		8.8312	7.6929	1
2	-7	5		39.2439	38.8806	1	3	-11	7		13.4529	13.1905	1
2	-7	7		32.2051	29.6181	1	3	-11	5		33.9392	33.6624	1
2	-7	9		12.4964	14.1548	1	3	-11	3		24.2200	22.8175	1
2	-6	6		17.4765	16.2410	1	3	-11	1		29.2006	29.0646	1
2	-6	4		8.6759	2.6179	1	3	-12	6		14.7662	9.6015	1
2	-6	2		14.4561	12.7581	1	3	-13	3		17.8198	16.5725	1
2	-5	1		91.4577	96.4797	1	3	-14	2		21.3807	19.9715	1
2	-5	3		55.6454	54.5431	1	3	-14	4		16.9057	16.4717	1
2	-5	5		62.8464	62.3373	1	3	-15	3		9.1644	4.0794	1
2	-5	7		60.9384	61.0815	1	3	-15	1		10.3122	9.9396	1
2	-5	9		37.2720	37.3891	1	3	-16	2		11.1896	9.2758	1
2	-4	10		28.3651	25.3991	1	4	-15	1		25.1335	26.4750	1
2	-4	8		37.8524	38.0457	1	4	-15	3		30.7023	29.0491	1
2	-4	6		44.3254	44.0265	1	4	-13	1		20.0596	20.3666	1
2	-4	4		47.5542	48.5561	1	4	-13	3		20.7942	19.6076	1
2	-4	2		54.6354	54.5016	1	4	-13	5		21.2137	20.2604	1
2	-3	5		19.0352	19.1602	1	4	-12	4		30.8763	30.4890	1
2	-3	6		8.3787	13.2491	1	4	-12	2		51.1349	48.9676	1
2	-3	7		24.1318	23.8270	1	4	-11	5		9.5382	5.4601	1
2	-3	9		9.6453	9.2868	1	4	-10	6		19.7191	19.1658	1
2	-2	10		27.9973	27.6196	1	4	-10	4		25.0666	23.5770	1
2	-2	8		30.0116	27.7511	1	4	-10	2		10.4844	8.9056	1
2	-2	6		51.0133	50.2217	1	4	-9	1		50.0507	48.5295	1
2	-2	4		62.7458	62.3114	1	4	-9	3		52.3318	52.8848	1
2	-1	3		75.5405	75.2240	1	4	-9	5		41.1293	41.6343	1
2	-1	5		50.5921	48.7792	1	4	-9	7		42.5484	41.9405	1
2	-1	7		34.4889	33.1299	1	4	-8	2		22.4625	20.6630	1
2	-1	9		40.8667	39.8294	1	4	-7	1		33.5590	32.4393	1

P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*
4	-7	3		11.0778	11.8975	1	5	-9	7		11.9135	12.0733	1
4	-7	7		12.9278	12.7113	1	5	-9	3		8.1318	0.9977	1
4	-6	8		32.5976	32.9128	1	5	-9	1		11.9518	10.1348	1
4	-6	7		9.0844	12.5347	1	5	-10	4		9.9707	8.8992	1
4	-6	6		45.1640	44.3780	1	5	-11	6		10.2830	7.3659	1
4	-6	5		8.1061	9.5001	1	5	-11	5		20.8284	19.0782	1
4	-6	4		60.7532	61.8321	1	5	-11	3		16.2105	16.6128	1
4	-6	2		54.8369	53.9405	1	5	-12	4		12.9258	14.5768	1
4	-5	1		19.9497	20.3022	1	5	-14	2		16.3093	16.9668	1
4	-5	2		6.8077	8.8690	1	5	-15	1		17.6651	18.4663	1
4	-5	9		9.6453	6.8791	1	6	-14	2		33.5055	31.8426	1
4	-4	9		9.4841	6.9039	1	6	-13	1		10.9500	11.0566	1
4	-4	8		12.4291	6.2863	1	6	-12	4		11.3936	9.5257	1
4	-4	6		14.2900	13.2187	1	6	-12	2		10.5947	9.1911	1
4	-4	5		8.6153	5.1276	1	6	-11	1		32.3233	32.6278	1
4	-4	4		17.5289	17.6936	1	6	-11	3		31.8113	30.1034	1
4	-4	2		6.3143	7.1139	1	6	-11	5		27.1160	27.0628	1
4	-3	1		108.5367	111.0851	1	6	-10	4		19.1290	20.5608	1
4	-3	2		7.0953	21.2903	1	6	-10	2		25.1998	24.8256	1
4	-3	3		73.6273	77.1212	1	6	-9	2		10.6496	1.5515	1
4	-3	5		60.1341	59.8935	1	6	-9	3		13.5233	11.1688	1
4	-3	7		46.8908	45.7154	1	6	-9	5		9.4061	5.3199	1
4	-3	9		43.7650	44.0218	1	6	-8	6		41.9622	40.6490	1
4	-2	9		9.2272	6.2540	1	6	-8	4		35.8488	34.7548	1
4	-2	8		8.6564	11.3011	1	6	-8	2		38.9660	39.1574	1
4	-2	4		11.2847	11.1325	1	6	-7	1		21.6708	22.6856	1
4	-2	2		30.7596	29.8536	1	6	-7	2		8.0450	15.2888	1
4	-1	1		5.6470	5.8206	1	6	-7	3		31.2209	29.0291	1
4	-1	3		12.7750	11.4653	1	6	-7	5		16.4733	18.2384	1
4	-1	5		26.7687	24.9381	1	6	-7	7		27.7474	28.2997	1
4	-1	8		9.2348	5.5892	1	6	-6	4		8.9159	7.2079	1
4	-1	9		11.8839	9.1717	1	6	-6	3		10.0759	6.9661	1
4	0	8		54.2265	53.0766	1	6	-6	2		12.5807	12.0847	1
4	0	6		73.3513	73.6541	1	6	-5	1		56.8246	57.6641	1
4	0	4		80.6847	82.8984	1	6	-5	3		62.3197	63.3715	1
4	0	2		113.4393	118.4314	1	6	-5	5		36.5380	36.7817	1
4	0	1		6.3733	19.2841	1	6	-5	7		26.5691	25.3038	1
5	-1	3		16.0473	18.8565	1	6	-4	8		16.9214	17.0124	1
5	-1	1		16.1756	17.4864	1	6	-4	6		26.2630	24.5390	1
5	-2	2		13.9723	14.3671	1	6	-4	4		35.0324	36.1809	1
5	-2	4		12.7281	9.6991	1	6	-4	2		41.8093	41.8766	1
5	-2	6		8.4037	1.2075	1	6	-3	1		19.0230	19.6225	1
5	-3	9		14.7575	10.8399	1	6	-3	3		27.1877	27.5951	1
5	-3	5		18.2627	15.8956	1	6	-3	5		12.3417	10.9365	1
5	-3	3		15.8789	15.5485	1	6	-3	8		10.4534	8.4737	1
5	-3	1		11.7518	12.3204	1	6	-2	8		33.4992	35.1490	1
5	-4	6		22.2290	24.2949	1	6	-2	6		30.9325	28.7853	1
5	-4	8		9.7986	9.8554	1	6	-2	4		32.5472	32.2611	1
5	-5	7		13.9944	13.3266	1	6	-2	2		39.0611	38.1001	1
5	-5	5		8.5444	5.2342	1	6	-1	1		50.6449	50.8442	1
5	-5	1		11.4431	10.3493	1	6	-1	3		26.1221	27.2282	1
5	-6	2		32.4749	32.3097	1	6	-1	5		38.3883	36.6122	1
5	-7	6		10.3924	9.9062	1	6	-1	7		22.1752	22.0746	1
5	-8	2		24.1857	23.8550	1	6	0	6		25.5859	25.7302	1
5	-8	4		9.6660	10.9833	1	6	0	4		12.2469	7.5384	1

P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*
6	0	2		8.2888	4.8103	1	9	-11	1		15.0913	17.8430	1
7	-1	3		13.4455	13.2238	1	10	-8	2		31.8361	32.4961	1
7	-1	1		7.6195	1.8142	1	10	-7	1		14.7044	16.8890	1
7	-2	2		9.5647	6.3505	1	10	-7	3		12.2977	18.6645	1
7	-2	4		9.4066	8.1170	1	10	-5	3		12.1048	15.1362	1
7	-3	7		11.6003	11.4951	1	10	-5	1		25.9211	23.7637	1
7	-3	2		7.8988	7.9378	1	10	-4	2		12.9017	14.3823	1
7	-3	1		19.1021	18.7389	1	10	-2	4		24.8797	24.4467	1
7	-4	1		7.5410	24.9220	1	10	-2	3		10.7941	19.7178	1
7	-4	2		11.3229	9.1521	1	10	-2	2		18.3065	20.9707	1
7	-5	5		10.2907	9.8047	1	10	-1	3		15.7365	16.9894	1
7	-5	1		10.1846	2.5196	1	10	-1	1		18.7433	17.8944	1
7	-6	4		19.3316	17.7407	1	10	0	4		11.1379	12.2419	1
7	-6	6		10.2887	8.2565	1	10	0	2		24.1616	25.4610	1
7	-8	2		14.9583	14.5905	1	10	0	1		9.1958	9.8759	1
7	-8	4		21.8277	22.3390	1	11	-3	1		8.8715	3.6793	1
7	-8	6		11.3158	12.5087	1	11	-7	1		8.8883	5.8294	1
7	-11	3		14.5621	15.1582	1	11	-8	0		14.2912	14.7367	1
7	-11	1		24.7763	24.8804	1	12	-3	1		20.3766	22.1931	1
7	-13	2		8.4348	17.7717	1	0	-17	-1		9.3378	5.2006	1
8	-12	2		18.3240	22.1851	1	0	-16	-2		14.1317	14.7535	1
8	-10	2		19.4524	18.1456	1	0	-16	-4		20.8274	22.2325	1
8	-9	1		30.2496	30.3842	1	0	-15	-5		24.3438	23.5838	1
8	-9	3		28.9956	28.8398	1	0	-15	-3		41.8891	42.5145	1
8	-8	4		11.2207	9.3987	1	0	-15	-1		39.3911	39.5705	1
8	-7	3		10.8391	10.1390	1	0	-14	-4		9.7266	3.7124	1
8	-7	5		15.0443	14.0125	1	0	-13	-7		18.6608	21.0830	1
8	-6	4		23.0863	24.6827	1	0	-13	-5		18.4326	18.2075	1
8	-6	2		36.0257	37.4023	1	0	-13	-3		30.4232	29.9767	1
8	-6	1		8.4071	23.9412	1	0	-13	-1		22.6122	23.4702	1
8	-5	5		9.3899	9.2490	1	0	-12	-2		48.0285	47.4200	1
8	-4	3		8.9927	7.2209	1	0	-12	-4		57.0507	55.6743	1
8	-3	1		44.2412	44.6007	1	0	-12	-6		49.8124	29.2608	1
8	-3	3		41.3165	41.5226	1	0	-12	-8		30.3973	30.1820	1
8	-3	5		39.4146	39.4390	1	0	-11	-1		9.4835	7.5047	1
8	-2	4		13.1814	14.1346	1	0	-10	-2		29.4089	29.6795	1
8	-2	2		11.3523	5.9732	1	0	-10	-4		13.3222	13.1323	1
8	-1	1		19.3849	21.7477	1	0	-10	-8		20.8940	21.0618	1
8	-1	2		10.3866	7.2972	1	0	-9	-9		36.2906	38.4259	1
8	-1	4		10.2158	12.0906	1	0	-9	-7		42.0373	41.3439	1
8	0	6		21.3279	22.9834	1	0	-9	-5		52.4283	53.1639	1
8	0	4		46.5504	46.0743	1	0	-9	-3		48.8396	47.7666	1
8	0	2		50.8244	52.8036	1	0	-9	-1		78.9017	82.0350	1
9	-2	1		8.5546	17.7416	1	0	-8	-1		13.3184	1.7707	1
9	-2	4		8.9825	2.7934	1	0	-8	-4		9.5680	6.3663	1
9	-3	5		9.3599	7.7324	1	0	-8	-5		7.3680	8.4361	1
9	-3	1		22.6549	22.1792	1	0	-8	-6		15.4988	12.4225	1
9	-4	2		12.5862	14.8294	1	0	-8	-10		11.6828	8.9329	1
9	-5	5		9.2816	4.0600	1	0	-7	-7		11.9301	9.7591	1
9	-5	3		11.1926	7.3269	1	0	-7	-5		37.9546	38.2322	1
9	-6	4		11.8828	9.2884	1	0	-7	-1		8.6029	6.9990	1
9	-8	2		9.3668	0.5531	1	0	-6	-2		103.1268	103.4142	1
9	-9	3		11.9361	12.5407	1	0	-6	-5		6.8709	5.9803	1
9	-9	1		10.0528	9.7994	1	0	-6	-4		78.3691	77.9040	1
9	-10	2		10.1336	6.7216	1	0	-6	-10		34.5994	33.5609	1

P <sub>21</sub> /a	h	k	l	(obs)	F(calc)	SF*	P <sub>21</sub> /a	h	k	l	F(obs)	F(calc)	SF*
0	-6	-6		55.6324	54.0568	1							
0	-5	-7		9.7667	8.4236	1	1	-11	-5		13.8915	15.1321	1
0	-6	-8		56.5477	56.2984	1	1	-11	-7		19.6928	17.0974	1
0	-5	-5		14.1274	14.8362	1	1	-11	-9		27.4000	27.4271	1
0	-5	-3		30.0291	28.4697	1	1	-12	-5		8.0879	10.7663	1
0	-4	-6		7.7350	5.9370	1	1	-12	-4		15.7612	15.6520	1
0	-4	-8		14.6679	14.2534	1	1	-12	-1		9.0927	3.0835	1
0	-4	-10		10.9299	12.8925	1	1	-13	-1		13.1177	14.0476	1
0	-3	-11		34.7129	34.2141	1	1	-13	-7		15.8676	13.1606	1
0	-3	-9		48.4532	49.3260	1	1	-14	-6		16.8121	18.9006	1
0	-3	-7		72.2182	73.0757	1	1	-14	-4		16.7177	17.1875	1
0	-3	-5		102.9614	100.7988	1	1	-14	-2		21.5546	21.0460	1
0	-3	-3		144.1054	142.8747	1	1	-14	0		19.2855	19.8997	1
0	-2	-4		32.1149	20.8062	1	1	-15	-1		11.5076	12.7845	1
0	-2	-6		26.8658	25.6971	1	1	-15	-3		19.7660	17.6380	1
0	-1	-9		17.8735	16.9043	1	1	-15	-5		16.2526	14.3320	1
0	-1	-7		18.4332	16.1866	1	1	-16	-4		16.1757	14.9247	1
0	0	-4		112.0368	106.0582	1	1	-16	-2		17.9233	16.0855	1
0	0	-6		93.1248	91.9820	1	1	-16	0		11.9385	10.4560	1
0	0	-7		8.9107	14.7104	1	1	-17	-1		15.7757	16.6823	1
0	0	-8		62.2521	60.6886	1	1	-17	-2		9.0174	8.2796	1
0	0	-10		65.1120	65.0154	1	2	-17	-1		27.5163	26.9386	1
1	-1	-5		24.5856	22.1712	1	2	-16	0		13.6474	13.0086	1
1	-2	-10		14.3629	8.1214	1	2	-16	-4		16.9065	14.2249	1
1	-2	-8		14.3739	12.1982	1	2	-14	0		39.5340	38.7670	1
1	-2	-6		11.3358	11.2310	1	2	-14	-2		35.5199	35.3185	1
1	-2	-4		7.8178	7.2050	1	2	-14	-4		43.0095	41.7272	1
1	-3	-7		7.8258	9.1808	1	2	-14	-6		22.7139	22.2776	1
1	-3	-9		23.2490	24.6365	1	2	-13	-7		18.5920	17.7948	1
1	-4	-10		8.5157	7.8816	1	2	-13	-3		15.0626	14.0384	1
1	-4	-6		23.9763	24.0860	1	2	-13	-1		16.2048	17.7046	1
1	-4	-4		23.6982	23.6041	1	2	-12	0		8.4499	6.8507	1
1	-5	-3		18.5727	17.0838	1	2	-12	-2		20.4312	20.1192	1
1	-5	-7		16.9449	15.7039	1	2	-12	-4		10.5290	8.5106	1
1	-6	-8		8.4242	2.3240	1	2	-12	-6		9.1935	0.8876	1
1	-6	-6		20.6267	21.8755	1	2	-12	-7		8.2019	2.5800	1
1	-6	-4		26.0481	26.3194	1	2	-11	-9		31.6418	32.5708	1
1	-6	-2		36.7121	37.1795	1	2	-11	-7		41.3906	40.2990	1
1	-6	0		14.1096	13.5761	1	2	-11	-5		46.2159	46.7240	1
1	-7	-3		10.0909	9.1838	1	2	-11	-4		8.0817	8.7741	1
1	-7	-10		9.9392	3.0729	1	2	-11	-3		46.2857	46.6476	1
1	-8	-10		9.4701	6.7676	1	2	-11	-1		46.8949	48.0086	1
1	-8	-6		20.3317	18.9752	1	2	-10	0		28.4909	28.8064	1
1	-8	-4		30.2408	30.1772	1	2	-10	-2		45.5148	45.2845	1
1	-8	-2		33.9570	32.4790	1	2	-10	-4		26.8732	26.7824	1
1	-8	0		15.1099	14.9856	1	2	-10	-6		19.5491	20.9274	1
1	-9	-1		20.3958	21.3850	1	2	-10	-8		17.1404	17.6117	1
1	-9	-3		8.3989	3.2123	1	2	-10	-9		9.4235	4.7282	1
1	-9	-5		7.8949	5.4919	1	2	-10	-10		16.8034	14.9400	1
1	-9	-7		14.9539	13.9948	1	2	-9	-7		18.9538	18.7424	1
1	-9	-9		8.4662	5.7284	1	2	-9	-3		7.2004	3.3855	1
1	-10	-4		15.1654	15.1061	1	2	-9	-1		7.9007	6.3305	1
1	-10	0		10.5925	12.5893	1	2	-8	0		72.6288	71.7369	1
1	-11	-1		16.1028	16.7743	1	2	-8	-2		85.5932	86.5235	1
1	-11	-3		23.0985	24.4142	1	2	-8	-4		54.3195	53.8205	1
							2	-8	-6		62.3243	63.8495	1



P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*
2	-8	-8		55.0974	54.4403	1	3	-6	-10		8.3803	9.7018	1
2	-8	-9		8.7786	12.3695	1	3	-6	-8		11.6242	13.5653	1
2	-8	-10		28.4595	28.3241	1	3	-6	-4		7.0082	8.6663	1
2	-7	-11		19.7397	18.8374	1	3	-6	-2		43.7945	44.9993	1
2	-7	-9		38.0600	37.5830	1	3	-6	0		22.4677	22.6064	1
2	-7	-7		36.5185	35.3347	1	3	-7	-3		7.2434	2.3611	1
2	-7	-5		56.1896	57.2199	1	3	-8	-10		16.6539	16.6671	1
2	-7	-3		36.0126	34.9608	1	3	-8	-8		13.1665	14.7531	1
2	-7	-1		32.9302	31.4895	1	3	-8	-4		15.0984	16.6526	1
2	-6	0		18.0040	17.6843	1	3	-8	-2		35.8947	36.7819	1
2	-6	-4		21.7543	21.7216	1	3	-8	0		32.2386	31.7307	1
2	-6	-5		6.4317	6.2807	1	3	-9	-1		7.0527	3.2893	1
2	-6	-10		11.5010	9.9429	1	3	-9	-3		9.0436	12.4512	1
2	-5	-11		39.4139	39.6802	1	3	-9	-5		8.3168	6.6412	1
2	-5	-9		44.6224	43.4782	1	3	-9	-7		11.1186	12.7425	1
2	-5	-7		40.3600	39.0921	1	3	-10	-8		9.0155	9.8911	1
2	-5	-5		77.0776	78.1616	1	3	-10	-5		7.4880	9.5486	1
2	-5	-3		113.1567	111.5497	1	3	-10	-3		8.3521	16.8103	1
2	-5	-1		114.8504	112.2977	1	3	-10	-2		7.3433	6.5127	1
2	-4	-4		69.1100	66.7080	1	3	-10	-1		8.2740	16.7424	1
2	-4	-6		43.1793	42.0379	1	3	-10	0		14.1011	12.1559	1
2	-4	-8		32.3241	32.9573	1	3	-11	-1		19.3178	20.1926	1
2	-4	-10		30.6867	30.0350	1	3	-11	-2		9.1205	2.5114	1
2	-4	-12		28.7095	27.1585	1	3	-11	-3		13.0412	13.8834	1
2	-3	-11		10.1512	10.5616	1	3	-11	-5		40.1089	39.7816	1
2	-3	-9		8.0772	10.2407	1	3	-11	-7		22.5410	22.2040	1
2	-3	-8		8.5393	10.0674	1	3	-12	-5		10.6365	3.9195	1
2	-3	-5		25.8807	25.4524	1	3	-12	-4		9.5466	8.5659	1
2	-2	-4		86.6033	83.3679	1	3	-12	0		14.8129	14.7561	1
2	-2	-6		68.7297	66.8244	1	3	-13	-3		8.4112	5.2379	1
2	-2	-8		51.2402	49.9536	1	3	-13	-6		10.0459	15.8827	1
2	-2	-10		39.2453	39.2011	1	3	-13	-7		11.7823	9.9172	1
2	-2	-12		15.6136	16.1403	1	3	-14	-6		12.5709	12.6844	1
2	-1	-11		27.4153	27.5458	1	3	-14	-4		17.4056	17.8056	1
2	-1	-9		29.3477	27.5988	1	3	-14	-2		24.9895	26.1181	1
2	-1	-7		55.6776	55.3107	1	3	-14	0		19.5184	19.2648	1
2	-1	-5		43.7718	41.4564	1	3	-15	-1		15.9234	16.7219	1
2	0	-6		46.8591	46.6799	1	3	-15	-3		8.8144	11.0928	1
2	0	-8		37.0987	36.3445	1	3	-16	-4		11.1919	7.3898	1
3	-1	-11		15.7914	14.5057	1	3	-16	-3		8.6505	11.1238	1
3	-2	-6		16.2153	16.9586	1	3	-16	-2		16.2523	14.6947	1
3	-3	-3		8.3709	8.6253	1	3	-16	0		11.6235	11.2635	1
3	-3	-5		46.7888	47.7906	1	4	-16	0		19.3581	18.8054	1
3	-3	-7		15.0601	13.2786	1	4	-16	-2		17.4463	19.2000	1
3	-4	-10		11.4453	9.2369	1	4	-16	-4		19.0216	18.8261	1
3	-4	-8		17.3681	18.7743	1	4	-15	-5		36.1075	35.9753	1
3	-4	-6		9.1332	8.5025	1	4	-15	-3		29.0541	28.5173	1
3	-4	-4		15.1180	15.1166	1	4	-15	-1		37.5499	37.3401	1
3	-4	-2		19.8226	18.9263	1	4	-14	-4		15.6545	14.8908	1
3	-4	0		30.5189	29.2528	1	4	-14	-5		9.3123	5.1729	1
3	-5	-1		7.4153	6.0434	1	4	-13	-7		21.8372	21.8618	1
3	-5	-3		23.1685	22.4890	1	4	-13	-5		23.3766	22.1097	1
3	-5	-7		14.5326	13.2758	1	4	-13	-3		15.4250	19.5985	1
3	-5	-8		7.9105	2.7538	1	4	-13	-1		29.0663	30.0385	1
3	-6	-11		10.3055	10.0286	1	4	-12	0		54.2293	54.1246	1

P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*
4	-12	-2		45.1764	45.5895	1	4	-2	-10		14.8072	14.6157	1
4	-12	-4		35.7599	37.3956	1	4	-1	-11		13.7051	15.3126	1
4	-12	-6		30.3565	31.3132	1	4	-1	-7		22.3336	21.6845	1
4	-12	-8		37.2803	37.4620	1	4	-1	-5		29.4419	29.0410	1
4	-11	-7		8.3319	0.5566	1	4	-1	-3		9.3771	6.5121	1
4	-10	0		14.1214	15.0599	1	4	0	0		86.3903	83.1711	1
4	-10	-2		18.7598	18.8611	1	4	0	-4		159.0786	162.1964	1
4	-10	-4		22.9655	23.5347	1	4	0	-6		85.4354	83.7303	1
4	-10	-6		26.5202	27.9983	1	4	0	-8		69.6268	68.7201	1
4	-10	-8		9.7394	9.2391	1	4	0	-10		46.4435	45.0159	1
4	-10	-10		9.1661	7.6724	1	4	0	-12		34.2716	32.1453	1
4	-9	-11		22.3707	20.1654	1	5	-1	-1		13.1545	13.2281	1
4	-9	-9		35.6355	35.4353	1	5	-1	-2		6.0056	16.8306	1
4	-9	-7		36.4571	37.9811	1	5	-1	-3		17.3807	16.7977	1
4	-9	-5		55.0698	54.8438	1	5	-1	-5		10.2201	11.1870	1
4	-9	-3		66.9834	68.2485	1	5	-1	-7		17.1610	17.0520	1
4	-9	-1		38.6807	39.0145	1	5	-2	-12		10.2352	6.9498	1
4	-8	-2		11.2284	10.7886	1	5	-2	-10		12.0406	10.6374	1
4	-8	-4		25.2273	26.8306	1	5	-2	-8		9.2680	5.2144	1
4	-8	-6		8.9832	1.2517	1	5	-2	-4		10.6903	10.6537	1
4	-8	-8		12.5027	9.5875	1	5	-2	-2		18.6360	18.7322	1
4	-8	-6		8.7794	1.2517	1	5	-2	0		15.4887	14.6526	1
4	-7	-9		25.5665	27.5740	1	5	-3	-1		37.2567	36.4902	1
4	-7	-5		7.3899	3.3644	1	5	-3	-3		34.2312	35.5031	1
4	-7	-3		17.7961	18.3345	1	5	-3	-5		11.9158	11.0546	1
4	-7	-1		9.3422	9.1273	1	5	-3	-7		16.3589	18.7488	1
4	-6	0		82.6740	82.6709	1	5	-3	-9		8.6320	3.8957	1
4	-6	-2		75.7698	76.2352	1	5	-4	-8		8.7294	9.9384	1
4	-6	-4		54.9994	55.2867	1	5	-4	-7		8.6670	13.4649	1
4	-6	-6		65.4949	68.0786	1	5	-4	-5		5.8140	11.9620	1
4	-6	-8		42.6801	43.2401	1	5	-4	-4		37.7765	38.5638	1
4	-6	-10		37.0997	36.4155	1	5	-5	-1		10.5091	10.1596	1
4	-6	-11		11.1331	18.0322	1	5	-5	-3		8.0976	6.7319	1
4	-6	-12		33.3520	33.5920	1	5	-5	-5		7.7354	10.4235	1
4	-5	-11		10.4827	7.3566	1	5	-5	-7		15.1450	13.9275	1
4	-5	-7		11.2981	8.5965	1	5	-5	-11		8.9054	1.5120	1
4	-5	-3		8.8593	8.2633	1	5	-6	-10		17.0810	17.5754	1
4	-5	-1		35.0041	35.0427	1	5	-6	-8		18.5096	20.3737	1
4	-4	-2		16.7762	16.6575	1	5	-6	-6		13.9373	13.8373	1
4	-4	-4		23.8948	23.8111	1	5	-6	-4		10.7353	13.8557	1
4	-4	-6		20.9348	19.5638	1	5	-6	0		28.7992	28.6931	1
4	-4	-8		10.0725	6.8236	1	5	-8	-10		11.9082	10.6302	1
4	-4	-12		14.0279	9.8208	1	5	-8	-8		15.2203	15.6285	1
4	-3	-11		46.2670	46.6249	1	5	-8	-6		8.4506	12.4530	1
4	-3	-9		57.5850	56.6746	1	5	-8	0		21.1776	22.6633	1
4	-3	-7		72.2687	70.9000	1	5	-9	-1		8.5401	7.5910	1
4	-3	-5		75.4260	77.2357	1	5	-9	-3		17.6558	18.2081	1
4	-3	-3		91.8497	90.5544	1	5	-9	-5		17.5355	19.4795	1
4	-3	-1		136.3747	132.6346	1	5	-9	-11		12.0852	7.0083	1
4	-2	0		26.9277	25.1517	1	5	-10	-4		12.7099	14.8339	1
4	-2	-2		16.6401	14.2596	1	5	-10	-2		9.2998	2.6869	1
4	-2	-4		6.9830	3.8802	1	5	-10	-1		8.9113	6.7433	1
4	-2	-6		11.9345	13.3639	1	5	-11	-1		25.1679	25.9876	1
4	-2	-8		18.1462	17.0221	1	5	-11	-3		25.3086	26.2520	1
4	-2	-9		8.5357	3.9012	1	5	-11	-5		12.1250	13.9739	1

$P_{21}/a$	h	k	l	$F_{(obs)}$	$F_{(calc)}$	SF*	$P_{21}/a$	h	k	l	$F_{(obs)}$	$F_{(calc)}$	SF*
5	-11	-7		13.6211	16.2979	1	6	-6	-10		10.8181	5.3577	1
5	-12	-6		12.4886	12.4402	1	6	-5	-11		22.6188	20.6903	1
5	-12	-2		18.9934	19.6706	1	6	-5	-9		42.2493	42.3680	1
5	-13	-3		14.7433	14.7565	1	6	-5	-7		60.1917	61.1680	1
5	-13	-4		9.1157	4.4746	1	6	-5	-5		52.3808	54.1246	1
5	-13	-5		10.5890	12.0639	1	6	-5	-3		54.3475	56.4467	1
5	-14	-6		11.1086	7.6576	1	6	-5	-1		48.2660	47.9616	1
5	-14	0		13.3064	14.0455	1	6	-4	0		40.9197	41.5129	1
5	-15	0		8.8161	10.8314	1	6	-4	-2		33.5390	33.7823	1
5	-15	-1		9.9350	11.8975	1	6	-4	-4		38.5500	38.8719	1
5	-16	-2		11.6954	7.0384	1	6	-4	-6		42.5018	43.9803	1
6	-15	-3		11.5785	9.8970	1	6	-4	-8		33.4178	33.2043	1
6	-14	0		17.2333	17.5669	1	6	-4	-10		24.9749	22.7094	1
6	-14	-2		23.0676	23.5872	1	6	-4	-12		17.0674	15.9749	1
6	-14	-4		20.8761	22.1567	1	6	-3	-9		11.1768	11.4315	1
6	-14	-6		24.7189	24.9375	1	6	-3	-7		22.8747	24.5625	1
6	-13	-5		13.7790	13.1326	1	6	-3	-5		15.9895	15.9968	1
6	-13	-3		8.3103	5.4130	1	6	-3	-3		13.5895	13.9766	1
6	-13	-1		11.8809	11.3944	1	6	-3	-1		6.9572	10.8467	1
6	-12	0		9.6849	5.2744	1	6	-2	-2		80.9368	82.1982	1
6	-12	-6		9.9229	11.0817	1	6	-2	0		44.0147	44.4738	1
6	-12	-7		14.0655	8.9042	1	6	-2	-6		27.7954	28.7173	1
6	-11	-9		26.6262	26.3971	1	6	-2	-4		52.2840	53.8268	1
6	-11	-7		30.1624	30.2432	1	6	-2	-8		35.4547	37.1340	1
6	-11	-5		31.3797	32.5477	1	6	-2	-10		28.4193	27.5444	1
6	-11	-3		40.5661	40.9720	1	6	-2	-12		30.3084	30.3806	1
6	-11	-1		40.6286	42.4058	1	6	-1	-11		27.8553	28.0219	1
6	-10	0		23.6578	23.0902	1	6	-1	-10		9.2031	16.0098	1
6	-10	-4		19.1607	19.0802	1	6	-1	-9		27.1202	26.7043	1
6	-10	-6		24.7072	25.4920	1	6	-1	-7		31.1184	31.2074	1
6	-10	-8		17.1873	17.1019	1	6	-1	-5		55.9052	56.9536	1
6	-10	-10		14.3959	15.5967	1	6	-1	-3		27.2885	26.5964	1
6	-9	-7		9.5813	10.8319	1	6	-1	-1		44.9069	44.1495	1
6	-9	-5		9.4557	7.2769	1	6	0	0		49.3678	50.6687	1
6	-9	-3		9.5292	3.4124	1	6	0	-2		33.3411	35.1043	1
6	-9	-2		7.6473	2.3535	1	6	0	-4		35.7119	37.6176	1
6	-9	-1		12.8498	10.9818	1	6	0	-6		16.1664	19.2020	1
6	-8	0		63.1719	64.1585	1	6	0	-10		19.7464	22.5206	1
6	-8	-1		7.1540	17.7666	1	6	0	-12		12.6528	12.1289	1
6	-8	-2		48.3816	50.2619	1	7	-1	-1		19.0224	20.5603	1
5	-8	-4		55.2182	57.4885	1	7	-1	-5		10.0227	9.2810	1
6	-8	-6		47.4525	49.5765	1	7	-1	-7		9.8288	12.3177	1
6	-8	-7		9.1025	22.7656	1	7	-2	-6		21.0936	21.7725	1
6	-8	-8		29.0449	28.0410	1	7	-3	-1		9.7886	10.9448	1
6	-8	-10		37.7824	39.3087	1	7	-3	-3		25.9362	26.7107	1
6	-7	-11		22.4453	18.7179	1	7	-3	-7		7.7204	0.6348	1
6	-7	-9		25.0330	23.7244	1	7	-3	-9		20.8525	20.2728	1
6	-7	-7		22.8199	23.2445	1	7	-4	-11		9.4614	15.4589	1
6	-7	-5		16.2136	17.2906	1	7	-4	-8		9.3670	9.5547	1
6	-7	-3		53.6416	56.2541	1	7	-4	-4		15.5617	15.9522	1
6	-7	-2		7.2504	21.9603	1	7	-4	-2		10.8795	9.6045	1
6	-7	-1		42.4635	43.6158	1	7	-4	0		19.4400	21.0045	1
6	-6	-1		8.1767	0.6047	1	7	-5	-1		15.7896	16.3555	1
6	-6	-2		13.8017	14.2387	1	7	-5	-3		8.2499	9.0019	1
6	-6	-8		12.8880	11.0123	1	7	-5	-11		10.6898	8.9931	1

P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub> /a	h	k	l	F(obs)	F(calc)	SF*
7	-6	-9		9.1973	4.4363	1	8	-7	-7		14.5370	15.8772	1
7	-6	-6		25.2634	26.9571	1	8	-7	-5		14.3685	11.9981	1
7	-8	-4		11.3001	16.7740	1	8	-7	-3		14.1258	13.6924	1
7	-6	0		8.7439	4.7298	1	8	-7	-1		10.4935	9.3261	1
7	-7	-3		7.5184	4.4318	1	8	-6	0		38.5146	39.3371	1
7	-8	-8		11.4710	10.0857	1	8	-6	-2		30.9304	32.7098	1
7	-8	-7		8.6396	15.2000	1	8	-6	-3		8.7177	30.3374	1
7	-8	-6		24.7876	22.8122	1	8	-6	-4		46.4601	47.8082	1
7	-8	-4		16.1931	16.7740	1	8	-6	-6		30.7852	31.9343	1
7	-8	-2		11.5473	9.4514	1	8	-6	-8		26.8422	27.3853	1
7	-9	-1		15.1644	15.2778	1	8	-6	-10		28.7330	30.6868	1
7	-10	-10		9.0241	10.2038	1	8	-5	-5		18.8810	20.7786	1
7	-10	-9		9.6686	9.4977	1	8	-5	-3		14.9931	14.9783	1
7	-10	-2		12.4677	13.0484	1	8	-4	0		14.3720	14.9247	1
7	-10	-1		8.4581	21.5261	1	8	-4	-1		7.9274	12.0160	1
7	-10	0		17.6931	16.7007	1	8	-4	-6		10.7615	6.3319	1
7	-11	-1		21.5973	20.8346	1	8	-4	-8		12.9256	11.6466	1
7	-11	-3		28.1922	28.5091	1	8	-4	-10		12.3514	12.7077	1
7	-11	-5		12.0797	8.5483	1	8	-4	-12		9.2294	5.9826	1
7	-11	-9		20.7643	22.5872	1	8	-3	-11		27.3853	26.5866	1
7	-12	-3		9.1261	3.0802	1	8	-3	-9		32.8919	33.8747	1
7	-13	-1		11.1259	9.2029	1	8	-3	-7		39.6234	41.2171	1
7	-13	-2		8.8315	13.5535	1	8	-3	-5		60.1306	61.2379	1
7	-13	-5		9.9877	7.4627	1	8	-3	-3		59.3181	61.8706	1
7	-14	-6		19.2171	15.1836	1	8	-3	-1		45.6579	45.5333	1
7	-14	-4		14.6392	14.7195	1	8	-2	0		8.2680	7.8426	1
7	-14	-3		9.4880	6.5317	1	8	-2	-2		12.1284	11.5495	1
7	-14	-2		16.4165	12.1809	1	8	-2	-3		7.7385	12.5250	1
7	-14	0		18.2678	16.8252	1	8	-2	-5		7.1472	16.6426	1
8	-14	-4		10.3738	8.4043	1	8	-2	-6		13.7450	13.3843	1
8	-13	-5		21.8652	22.1008	1	8	-2	-7		8.5780	4.9251	1
8	-13	-4		8.6486	3.5579	1	8	-2	-12		10.3124	10.8238	1
8	-13	-3		14.4954	17.8722	1	8	-1	-12		8.6059	9.0202	1
8	-13	-2		9.7313	7.7791	1	8	-1	-9		18.0633	18.4537	1
8	-13	-1		14.8019	14.2870	1	8	-1	-5		14.9614	14.8954	1
8	-12	0		20.1204	18.9405	1	8	-1	-3		10.4872	11.3295	1
8	-12	-2		30.8493	30.9689	1	8	0	0		66.7118	69.4327	1
8	-12	-4		33.3010	33.4470	1	8	0	-2		71.8016	74.0945	1
8	-12	-6		28.6897	28.6449	1	8	0	-4		37.1002	36.9247	1
8	-12	-8		15.7128	19.4697	1	8	0	-6		54.7143	56.4016	1
8	-11	-3		9.8880	1.6617	1	8	0	-8		58.4842	57.3027	1
8	-10	0		17.1250	18.4737	1	8	0	-10		39.5273	37.6694	1
8	-10	-2		10.9806	11.0044	1	8	0	-12		33.6809	35.1533	1
8	-10	-4		8.9783	12.0624	1	9	-1	-3		7.7319	5.5518	1
8	-10	-8		17.8245	16.7483	1	9	-1	-7		12.3473	14.9956	1
8	-9	-9		24.4150	23.2424	1	9	-1	-9		9.1602	11.3493	1
8	-9	-7		32.4445	34.5049	1	9	-2	-12		10.1316	10.1904	1
8	-9	-5		17.3322	20.1824	1	9	-2	-8		9.6483	10.9150	1
8	-9	-3		23.6924	24.4646	1	9	-2	-4		12.5342	11.8862	1
8	-9	-2		8.2493	24.8801	1	9	-2	-2		18.7875	19.1743	1
8	-9	-1		39.3947	41.7655	1	9	-3	-1		12.5092	10.0186	1
8	-8	0		12.0768	10.9474	1	9	-3	-4		8.6238	4.5387	1
8	-8	-2		18.8209	16.7791	1	9	-3	-5		19.9049	19.2661	1
8	-8	-6		10.1999	10.1447	1	9	-3	-7		12.6740	11.1701	1
8	-8	-8		10.7847	9.3487	1	9	-3	-9		12.8147	12.7785	1

$P_{21}/a$	h	k	l	F(obs)	F(calc)	SF*	$P_{21}/a$	h	k	l	F(obs)	F(calc)	SF*
9	-4	-8		17.7473	14.7019	1	10	-4	-2		23.1043	24.0455	1
9	-4	-7		8.4072	18.4382	1	10	-4	-4		21.9162	20.9820	1
9	-5	-2		8.3874	16.7500	1	10	-4	-6		12.7188	12.3098	1
9	-5	-3		8.4216	3.2569	1	10	-4	-7		8.2223	23.6175	1
9	-5	-4		9.2287	17.5833	1	10	-4	-8		14.8234	13.1606	1
9	-5	-5		14.9079	15.3952	1	10	-4	-10		14.2628	16.3795	1
9	-5	-9		8.9127	4.0111	1	10	-3	-11		14.2439	9.3491	1
9	-5	-11		12.3686	11.1336	1	10	-3	-5		9.7152	7.8843	1
9	-6	-6		9.5470	8.2437	1	10	-3	-3		12.9400	11.9789	1
9	-6	-4		19.9947	19.0185	1	10	-3	-2		9.2073	3.5575	1
9	-6	-2		25.5814	26.2450	1	10	-3	-1		18.0961	17.3239	1
9	-7	-6		8.1909	9.4351	1	10	-2	0		24.2248	23.4225	1
9	-7	-7		10.6196	6.2226	1	10	-2	-2		14.0864	13.5262	1
9	-7	-8		10.9200	13.0556	1	10	-2	-4		18.4897	19.0293	1
9	-8	-8		8.1614	4.1788	1	10	-2	-6		35.0228	36.3816	1
9	-8	-4		8.9667	11.0654	1	10	-2	-8		19.9966	20.4032	1
9	-8	-2		8.6264	11.5309	1	10	-2	-9		8.4342	26.8090	1
9	-8	-1		8.0802	14.5417	1	10	-2	-10		15.9903	13.9267	1
9	-9	-1		9.4323	6.1750	1	10	-1	-9		17.2659	20.7127	1
9	-9	-3		11.0832	7.7477	1	10	-7	-7		14.5546	25.0499	1
9	-9	-7		17.9211	14.1916	1	10	-1	-5		16.1972	12.8733	1
9	-10	-8		12.1108	13.4691	1	10	-1	-4		8.6775	22.2944	1
9	-10	-3		9.6901	15.2729	1	10	-1	-3		27.7853	28.8019	1
9	-11	-5		8.5453	10.9728	1	10	-1	-1		15.0661	13.8615	1
9	-12	-6		11.9970	12.2983	1	10	0	-2		10.5073	6.1138	1
9	-12	-5		11.1402	11.2439	1	10	0	-4		21.8581	19.3119	1
9	-12	-4		11.8557	11.7031	1	10	0	-6		16.2933	13.4295	1
9	-12	-1		8.3662	6.0644	1	10	0	-8		23.0867	22.8123	1
9	-12	0		11.5962	13.3969	1	11	-1	-5		15.3822	16.7800	1
9	-13	-4		7.7817	5.0155	1	11	-2	-11		10.0343	8.1276	1
10	-11	-7		20.3243	19.8054	1	11	-2	-10		10.2306	15.3659	1
10	-11	-5		21.4517	24.0803	1	11	-2	-8		9.2868	8.1081	1
10	-11	-3		16.7663	17.5453	1	11	-2	-4		10.6406	11.2879	1
10	-11	-1		16.3817	17.5001	1	11	-2	0		10.7837	9.1732	1
10	-10	-2		14.6035	17.4579	1	11	-3	-1		10.9058	6.4175	1
10	-10	-4		10.2782	11.0799	1	11	-3	-7		17.9442	16.4165	1
10	-10	-7		9.7565	22.5714	1	11	-4	-2		13.8693	13.2464	1
10	-8	0		20.6130	20.7507	1	11	-4	0		9.7866	8.5382	1
10	-8	-2		26.9580	27.5655	1	11	-5	-1		10.3008	9.9279	1
10	-8	-4		32.3634	32.8215	1	11	-5	-7		8.5135	9.2581	1
10	-8	-6		25.1884	23.8357	1	11	-5	-9		9.2477	0.7219	1
10	-8	-8		31.3708	33.0033	1	11	-6	-2		10.2873	7.6752	1
10	-7	-10		9.2716	21.2560	1	11	-6	-10		13.4431	13.0967	1
10	-7	-7		24.4029	25.0499	1	11	-7	-5		8.5055	10.7559	1
10	-7	-5		24.1157	24.3209	1	11	-7	-7		10.0872	10.1973	1
10	-7	-1		17.0288	16.1295	1	11	-8	-5		9.6911	11.1424	1
10	-6	-8		8.9723	4.9043	1	11	-8	-2		12.9200	9.0612	1
10	-6	-10		10.0612	0.8334	1	11	-9	-1		8.8171	6.2950	1
10	-5	-11		27.4325	28.2122	1	11	-9	-5		11.1111	7.6801	1
10	-5	-9		20.5655	19.7937	1	11	-10	-6		13.9904	13.3075	1
10	-5	-7		21.2611	21.5627	1	11	-10	-4		19.0213	19.6137	1
10	-5	-5		26.9749	27.4438	1	11	-10	-3		9.3729	18.5168	1
10	-5	-3		33.2353	34.0461	1	12	-8	-4		11.5122	12.4386	1
10	-5	-1		40.0785	41.1605	1	12	-8	-6		13.4123	8.7758	1
10	-4	0		19.0096	20.7633	1	12	-6	-2		17.5247	17.9003	1

$P_{21}/a$	h	k	l	$F_{(obs)}$	$F_{(calc)}$	SF*	$P_{21}/a$	h	k	l	$F_{(obs)}$	$F_{(calc)}$	SF*
12	-6	-4		12.1189	11.3804	1		0	0	2	187.5976	169.8391	2
12	-6	-6		11.9453	11.1032	1		0	0	1	13.3769	8.7834	2
12	-6	-7		11.4304	24.1895	1		1	-1	3	6.4431	5.6980	2
12	-6	-8		17.8355	16.5895	1		1	-1	2	4.4758	3.7762	2
12	-5	-9		12.4837	10.2567	1		1	-1	1	13.8962	10.8527	2
12	-5	-7		9.9141	8.0046	1		1	-1	0	8.2772	7.8114	2
12	-5	-5		12.1641	4.4165	1		1	-1	-3	70.7673	67.8255	2
12	-4	-4		10.8263	9.2188	1		1	-2	-2	17.8630	17.5642	2
12	-4	-8		9.1654	2.1820	1		1	-2	-1	5.6647	3.5183	2
12	-3	-9		24.3509	20.8643	1		1	-2	0	4.6455	2.8179	2
12	-3	-8		8.5425	31.5079	1		1	-2	2	47.6176	47.4853	2
12	-3	-7		24.5458	22.8189	1		1	-3	1	76.3176	83.8311	2
12	-3	-5		13.8837	14.3281	1		1	-3	-1	6.8706	5.4153	2
12	-3	-3		17.2460	18.4291	1		1	-4	-2	17.1503	18.3069	2
12	-3	-2		8.8572	26.1795	1		1	-4	0	73.9042	70.2203	2
12	-3	-1		22.2789	24.2014	1		1	-5	-1	35.5265	35.8215	2
12	-2	-2		10.2474	3.8014	1		2	-4	0	82.3323	80.3249	2
12	-2	-7		9.5485	13.6240	1		2	-4	-2	98.8030	99.2707	2
12	-1	-4		9.7163	12.6217	1		2	-3	-3	46.4722	48.4157	2
12	-1	-3		8.9800	11.4943	1		2	-3	-1	43.8819	44.3509	2
12	0	0		24.4041	22.5551	1		2	-3	1	29.1746	29.8704	2
12	0	-2		21.0890	21.4609	1		2	-2	2	103.9306	117.4788	2
12	0	-4		37.9110	38.2180	1		2	-2	0	116.5629	109.7194	2
12	0	-6		30.4214	29.9442	1		2	-2	-2	28.6097	33.2751	2
12	0	-8		11.1812	10.1246	1		2	-1	-3	89.2543	87.9412	2
12	0	-10		19.8168	19.2738	1		2	-1	-1	127.5448	128.1520	2
13	-1	-5		9.9356	8.8873	1		2	-1	1	34.4883	37.3123	2
13	-1	-8		9.9151	15.5347	1		2	0	2	65.9987	66.9127	2
13	-2	-8		10.4811	10.8751	1		2	0	0	37.2071	36.1049	2
13	-2	-6		15.2445	16.9699	1		2	0	-1	4.8920	3.7985	2
13	-3	-3		16.7823	18.5014	1		3	-1	1	31.4919	30.7387	2
13	-3	-8		9.3694	5.0023	1		3	-1	-1	65.5282	63.8515	2
13	-4	-8		10.4824	14.9417	1		3	-1	-3	12.7339	11.5613	2
13	-4	-7		8.7912	10.0497	1		3	-2	-3	5.1487	14.4815	2
13	-4	-2		9.9973	1.6293	1		3	-2	-2	36.5582	34.3573	2
13	-5	-3		10.3554	11.0647	1		3	-2	0	13.3218	14.3456	2
13	-5	-7		9.1872	11.8314	1		3	-3	-1	9.1073	9.6394	2
13	-6	-6		14.8241	14.9095	1		4	-1	-1	49.6819	49.8621	2
13	-6	-4		8.9798	3.1296	1		4	0	-2	120.9799	129.6116	2
0	-5	-1		17.2253	18.0377	2							
0	-5	1		17.4830	18.0379	2							
0	-4	2		28.7676	28.0632	2							
0	-4	1		4.4642	3.6669	2							
0	-4	0		40.3355	40.1313	2							
0	-4	-2		28.2346	28.0631	2							
0	-3	-1		131.9186	131.3434	2							
0	-3	1		126.8247	131.3435	2							
0	-2	3		6.2913	0.9969	2							
0	-2	2		12.0187	10.2558	2							
0	-2	0		14.5720	12.6506	2							
0	-2	-2		11.8711	10.2555	2							
0	-1	-3		61.8190	59.5685	2							
0	-1	-1		39.6328	36.7512	2							
0	-1	1		39.0007	36.7511	2							
0	-1	3		62.0178	59.5687	2							

P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*
5	0		6	8.2513	6.2823	1	0	-7		1	6.8007	10.1532	1
5	0		7	9.7105	7.5692	1	0	-7		3	8.2267	9.3770	1
5	0		9	10.1910	9.0043	1	0	-7		5	39.8014	37.8909	1
7	0		3	7.7907	12.8746	1	0	-7		6	10.4172	3.9126	1
3	0		-7	6.7950	9.5981	1	0	-6		11	9.4654	4.1869	1
3	0		-6	6.1620	4.8980	1	0	-6		10	33.4239	32.9642	1
5	0		-7	6.7411	8.6985	1	0	-6		8	58.1644	56.2501	1
5	0		-4	6.5106	6.3787	1	0	-6		6	55.9221	54.7841	1
7	0		-12	9.2967	8.3126	1	0	-6		4	76.8185	77.8148	1
7	0		-7	10.9936	17.4554	1	0	-6		2	104.6836	104.2045	1
7	0		-3	7.3077	8.2695	1	0	-6		0	75.9184	76.0725	1
7	0		0	11.2727	10.6946	1	0	-5		3	30.0771	27.6340	1
9	0		-10	8.5858	11.3950	1	0	-5		5	12.3698	14.4457	1
9	0		-8	9.5370	12.0713	1	0	-5		7	10.0069	8.1754	1
9	0		-1	7.5192	13.9974	1	0	-5		11	9.1235	8.1194	1
11	0		-9	9.3407	10.6517	1	0	-4		10	12.6673	13.0085	1
11	0		-8	8.6580	13.8711	1	0	-4		8	16.3510	14.7079	1
11	0		-1	9.8436	10.2887	1	0	-4		6	8.8987	7.1761	1
1	0		-1	4.4128	9.5448	2	0	-4		4	8.2181	9.0799	1
1	0		1	4.4646	3.4635	2	0	-3		3	146.0397	144.7525	1
1	0		2	5.1761	0.4823	2	0	-3		5	102.5300	101.2722	1
0	-16		4	21.1228	22.2200	1	0	-3		7	74.5913	72.8118	1
0	-16		2	14.4853	14.7389	1	0	-3		9	51.6456	49.7495	1
0	-16		0	22.3700	21.2447	1	0	-3		11	33.8697	34.5445	1
0	-15		1	38.9844	38.2691	1	0	-2		11	9.2360	3.8149	1
0	-15		3	44.2237	41.3620	1	0	-2		6	26.7473	25.7959	1
0	-15		5	26.6520	22.9606	1	0	-2		4	32.8542	30.6577	1
0	-14		4	9.5052	5.9995	1	0	-1		7	15.8440	16.8433	1
0	-14		0	18.4797	18.5321	1	0	-1		9	14.3461	17.2904	1
0	-13		1	22.9707	23.4107	1	1	-1		7	22.6709	22.2171	1
0	-13		3	29.4310	30.2162	1	1	-1		5	15.4882	16.3543	1
0	-13		5	18.7498	17.5507	1	1	-2		4	12.2418	13.3961	1
0	-13		7	19.9313	20.1938	1	1	-2		7	7.7865	8.4675	1
0	-12		8	29.3968	28.9480	1	1	-3		11	10.1992	7.3469	1
0	-12		6	49.8827	47.9687	1	1	-3		7	14.1235	14.1904	1
0	-12		4	58.6289	55.3410	1	1	-3		5	7.7256	8.3362	1
0	-12		2	47.5826	47.1049	1	1	-3		3	38.8671	35.4577	1
0	-12		0	48.3679	46.4593	1	1	-4		2	15.4121	15.5711	1
0	-11		1	9.3994	8.1084	1	1	-4		4	25.7180	26.7126	1
0	-10		9	9.5797	3.6229	1	1	-4		7	8.5007	3.6301	1
0	-10		8	21.0835	21.2700	1	1	-4		8	7.8547	2.3174	1
0	-10		4	13.0503	13.8167	1	1	-4		10	20.1798	19.9090	1
0	-10		2	29.1162	29.5562	1	1	-5		9	12.6233	10.6397	1
0	-10		0	28.7945	28.4066	1	1	-5		7	7.5582	6.5287	1
0	-9		1	79.8896	82.4728	1	1	-5		5	15.2930	15.5472	1
0	-9		3	50.1535	48.6516	1	1	-5		3	10.4820	8.7099	1
0	-9		5	53.8007	53.1986	1	1	-5		1	7.2233	5.6599	1
0	-9		7	42.9645	40.8118	1	1	-6		2	10.9194	12.3466	1
0	-9		-9	39.2114	37.0410	1	1	-6		4	27.0374	26.4802	1
0	-8		6	10.6529	13.3719	1	1	-6		6	24.6439	22.5884	1
0	-8		2	6.9223	6.2724	1	1	-6		7	7.5332	8.9157	1
0	-8		1	7.4729	5.1700	1	1	-6		8	12.1213	8.8480	1
0	-8		0	40.6529	40.6862	1	1	-8		2	7.0756	7.3451	1

P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*
1	-8	4		24.8116	24.3250	1	2	-5	5		62.6149	62.6835	1
1	-8	6		25.3260	24.9731	1	2	-5	7		60.6308	60.3379	1
1	-8	8		16.8107	15.8088	1	2	-5	9		37.0115	36.6356	1
1	-8	10		9.7750	8.4255	1	2	-4	10		28.1528	25.0485	1
1	-9	7		8.3237	3.7055	1	2	-4	8		37.5959	37.7618	1
1	-9	5		8.1823	8.0842	1	2	-4	6		44.0620	44.1641	1
1	-9	3		14.2300	11.9997	1	2	-4	4		47.3377	49.0191	1
1	-9	1		14.8911	14.9537	1	2	-4	2		54.5772	56.1033	1
1	-10	6		13.0420	9.6839	1	2	-3	5		18.8917	19.0909	1
1	-10	8		8.3077	9.0855	1	2	-3	6		8.3116	11.6308	1
1	-11	7		20.9198	19.6478	1	2	-3	7		23.9500	23.3689	1
1	-11	3		31.6978	30.5407	1	2	-3	9		9.5686	8.8104	1
1	-11	1		45.6371	43.2422	1	2	-2	10		27.7893	27.0025	1
1	-12	2		22.8676	20.3398	1	2	-2	8		29.7985	28.3955	1
1	-13	5		8.2600	5.7422	1	2	-2	6		50.7587	50.7414	1
1	-13	3		8.8447	10.3289	1	2	-2	4		62.6139	62.4475	1
1	-13	1		13.4693	13.3563	1	2	-1	3		75.7843	76.0826	1
1	-14	2		14.5158	14.4448	1	2	-1	5		50.3648	49.3577	1
1	-14	4		22.4496	20.1859	1	2	-1	7		34.2498	32.9223	1
1	-14	6		17.2599	17.2003	1	2	-1	9		40.5969	39.5658	1
1	-15	3		12.7784	7.6719	1	2	0	10		14.9212	14.2261	1
1	-15	5		17.8224	15.2057	1	2	0	8		14.0567	10.3112	1
1	-17	1		14.3026	7.9732	1	2	0	4		64.4410	63.4545	1
2	-16	3		10.9200	6.1607	1	3	-1	9		10.5785	12.2004	1
2	-16	2		20.0197	17.9100	1	3	-1	7		10.9179	10.7870	1
2	-16	1		9.1066	4.4880	1	3	-1	3		17.1143	15.8426	1
2	-15	1		16.4862	15.4147	1	3	-2	2		7.6395	5.5933	1
2	-14	4		20.0141	19.9545	1	3	-2	4		10.4825	8.7327	1
2	-14	2		29.4078	28.1311	1	3	-2	6		11.6325	12.1637	1
2	-13	1		14.0947	10.8782	1	3	-2	8		12.7095	5.6172	1
2	-13	3		19.9241	19.5777	1	3	-3	10		8.4664	2.6437	1
2	-13	5		14.4603	12.8853	1	3	-3	7		9.0873	4.2103	1
2	-11	1		54.5480	54.4440	1	3	-3	5		30.0190	29.1526	1
2	-11	3		51.7740	49.8280	1	3	-3	3		11.5354	9.9901	1
2	-11	5		39.4974	39.8404	1	3	-3	1		32.4363	29.3456	1
2	-11	7		32.3833	31.6626	1	3	-4	2		32.0244	32.4656	1
2	-10	8		25.9637	25.1918	1	3	-4	4		23.5894	24.4048	1
2	-10	6		23.2252	23.5918	1	3	-4	8		12.8435	10.4700	1
2	-10	4		28.3557	26.8747	1	3	-5	3		26.3017	25.7828	1
2	-10	2		19.3881	18.2839	1	3	-6	2		14.2993	14.8102	1
2	-9	3		23.9061	22.6563	1	3	-6	8		16.6392	18.1938	1
2	-8	8		39.9963	39.2895	1	3	-8	2		19.5439	19.3683	1
2	-8	6		41.0132	38.3855	1	3	-8	4		10.9349	9.5697	1
2	-8	4		73.5475	74.8795	1	3	-8	6		11.7083	13.2432	1
2	-8	2		71.4516	73.0648	1	3	-8	8		19.5224	20.3692	1
2	-7	1		79.5676	82.9627	1	3	-9	3		19.4365	18.9932	1
2	-7	3		49.8160	50.9364	1	3	-10	2		11.0479	11.5076	1
2	-7	5		38.9927	39.1700	1	3	-10	4		8.7622	9.3275	1
2	-7	7		31.9780	30.2066	1	3	-11	7		13.3466	12.5521	1
2	-7	9		12.3989	14.2512	1	3	-11	5		33.7410	32.5712	1
2	-6	6		17.3402	15.7608	1	3	-11	3		24.0358	22.3100	1
2	-6	4		8.6072	4.2724	1	3	-11	1		28.9852	28.3244	1
2	-6	2		14.3457	13.3023	1	3	-12	6		14.6507	10.6685	1
2	-5	1		92.0301	96.6227	1	3	-13	3		17.6823	16.7531	1
2	-5	3		55.4829	55.6757	1	3	-14	2		21.2147	19.1417	1



P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*
3	-14	4		16.7736	15.9872	1	4	0	4		80.6562	82.4754	1
3	-15	3		9.0916	4.9767	1	4	0	2		114.6787	119.1028	1
3	-15	1		10.2315	10.7460	1	4	0	1		6.3240	17.8066	1
3	-16	2		11.1015	9.7346	1	5	-1	3		15.9247	18.3313	1
4	-15	1		24.9431	25.4308	1	5	-1	1		16.0544	17.4883	1
4	-15	3		30.4742	28.2675	1	5	-2	2		13.8646	14.3040	1
4	-13	1		19.9054	19.9406	1	5	-2	4		12.6294	10.8665	1
4	-13	3		20.6321	18.6457	1	5	-2	6		8.3370	3.2566	1
4	-13	5		21.0541	20.9120	1	5	-3	9		14.6430	12.0224	1
4	-12	4		30.6500	29.8883	1	5	-3	5		18.1204	15.4713	1
4	-12	2		50.8232	48.2399	1	5	-3	3		15.7572	15.7416	1
4	-11	5		9.4640	8.6628	1	5	-3	1		11.6626	13.3336	1
4	-10	6		19.5660	18.5205	1	5	-4	6		22.0586	23.1549	1
4	-10	4		24.8808	23.9675	1	5	-4	8		9.7205	8.9498	1
4	-10	2		10.4039	11.4666	1	5	-5	7		13.8846	13.0954	1
4	-9	1		49.7763	48.9775	1	5	-5	5		8.4766	5.6005	1
4	-9	3		52.0281	51.9220	1	5	-5	1		11.3562	12.3491	1
4	-9	5		40.8503	40.7325	1	5	-6	2		32.2371	30.8390	1
4	-9	7		42.2662	41.4252	1	5	-7	6		10.3086	7.6553	1
4	-8	2		22.2971	21.4744	1	5	-8	2		24.0079	24.2524	1
4	-7	1		33.3297	32.2430	1	5	-8	4		9.5903	11.4625	1
4	-7	3		10.9921	12.7093	1	5	-9	7		11.8196	11.8298	1
4	-7	7		12.8277	13.5582	1	5	-9	3		8.0673	3.8300	1
4	-6	8		32.3578	31.7029	1	5	-9	1		11.8574	9.9699	1
4	-6	7		9.0117	10.8606	1	5	-10	4		9.8924	9.6382	1
4	-6	6		44.8728	43.7353	1	5	-11	6		10.2000	4.5640	1
4	-6	5		8.0418	9.0982	1	5	-11	5		20.6685	19.0009	1
4	-6	4		60.4968	61.8423	1	5	-11	3		16.0862	17.0225	1
4	-6	2		54.6014	54.4721	1	5	-12	4		12.8231	13.3547	1
4	-5	1		19.8031	20.4678	1	5	-14	2		16.1804	15.6910	1
4	-5	2		6.7588	13.7840	1	5	-15	1		17.5277	17.8169	1
4	-5	9		9.5686	6.6683	1	6	-14	2		33.2622	31.2101	1
4	-4	9		9.4099	8.6503	1	6	-13	1		10.8645	11.8231	1
4	-4	8		12.3314	7.7571	1	6	-12	4		11.3042	10.2920	1
4	-4	6		14.1792	13.7189	1	6	-12	2		10.5123	10.7223	1
4	-4	5		8.5471	5.9253	1	6	-11	1		32.0965	32.7761	1
4	-4	4		17.3937	17.2563	1	6	-11	3		31.5745	29.0347	1
4	-4	2		6.2647	7.6116	1	6	-11	5		26.9073	25.4631	1
4	-3	1		109.3829	110.8543	1	6	-10	4		18.9819	20.0815	1
4	-3	2		7.0340	16.4020	1	6	-10	2		25.0075	23.8447	1
4	-3	3		73.5731	77.2402	1	6	-9	2		10.5645	1.1285	1
4	-3	5		59.8935	60.4135	1	6	-9	3		13.4171	11.3155	1
4	-3	7		46.6058	45.6547	1	6	-9	5		9.3318	6.5626	1
4	-3	9		43.4716	43.0454	1	6	-8	6		41.6828	40.2847	1
4	-2	9		9.1531	4.5326	1	6	-8	4		35.6015	34.7112	1
4	-2	8		8.5888	11.8945	1	6	-8	2		38.6999	38.4073	1
4	-2	4		11.1949	10.1343	1	6	-7	1		21.5101	23.0249	1
4	-2	2		30.5614	30.0472	1	6	-7	2		7.9827	15.4316	1
4	-1	1		5.6030	6.8342	1	6	-7	3		30.9973	29.1184	1
4	-1	3		12.6763	11.8321	1	6	-7	5		16.3452	17.6247	1
4	-1	5		26.5754	25.0901	1	6	-7	7		27.5370	26.9669	1
4	-1	8		9.1614	5.6272	1	6	-6	4		8.8453	7.5424	1
4	-1	9		11.7900	9.2194	1	6	-6	3		9.9992	10.8069	1
4	0	8		53.9359	53.0062	1	6	-6	2		12.4814	11.6143	1
4	0	6		73.1042	72.5406	1	6	-5	1		56.5373	56.8170	1

P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*
6	-5	3		62.0174	62.1427	1	8	-3	5		39.1365	37.9255	1
6	-5	5		36.2883	36.4203	1	8	-2	4		13.0778	13.6359	1
6	-5	7		26.3723	25.2533	1	8	-2	2		11.2626	6.7625	1
6	-4	8		16.7904	16.9105	1	8	-1	1		19.2388	21.6028	1
6	-4	6		26.0687	24.6133	1	8	-1	2		10.3072	10.7249	1
6	-4	4		34.7914	35.5957	1	8	-1	4		10.1388	14.5292	1
6	-4	2		41.5508	41.7302	1	8	0	6		21.1667	22.5690	1
6	-3	1		18.8780	19.1815	1	8	0	4		46.2639	45.5448	1
6	-3	3		26.9855	26.6341	1	8	0	2		50.5226	51.4051	1
6	-3	5		12.2438	10.2234	1	9	-2	1		8.4827	12.5201	1
6	-3	8		10.3699	7.6312	1	9	-2	4		8.9112	3.9331	1
6	-2	8		33.2578	33.9475	1	9	-3	5		9.2885	11.2869	1
6	-2	6		30.7018	27.6837	1	9	-3	1		22.4853	22.4249	1
6	-2	4		32.3232	32.2960	1	9	-4	2		12.4875	14.4014	1
6	-2	2		38.8225	38.5751	1	9	-5	5		9.2095	8.0668	1
6	-1	1		50.4127	51.1132	1	9	-5	3		11.1052	9.1062	1
6	-1	3		25.9339	27.0179	1	9	-6	4		11.7893	9.7345	1
6	-1	5		38.1299	36.2259	1	9	-8	2		9.2938	6.8049	1
6	-1	7		22.0093	22.1940	1	9	-9	3		11.8925	12.8860	1
6	0	6		25.3939	24.9041	1	9	-9	1		9.9752	11.8016	1
6	0	4		12.1498	7.4942	1	9	-10	2		10.0533	7.1898	1
6	0	2		8.2229	4.9598	1	9	-11	1		14.9740	17.3671	1
7	-1	3		13.3398	12.7658	1	10	-8	2		31.6017	31.4353	1
7	-1	1		7.5591	3.7136	1	10	-7	1		14.5889	15.9906	1
7	-2	2		9.4890	6.7444	1	10	-7	3		12.2017	17.8582	1
7	-2	4		9.3320	8.0651	1	10	-5	3		12.0110	15.2910	1
7	-3	7		11.5094	11.7944	1	10	-5	1		25.7309	24.4700	1
7	-3	2		7.8410	13.6881	1	10	-4	2		12.8031	15.5845	1
7	-3	1		18.9620	20.1923	1	10	-4	4		24.6921	23.8954	1
7	-4	1		7.4729	16.5611	1	10	-2	3		10.7053	15.8998	1
7	-4	2		11.2334	9.1641	1	10	-2	2		18.1656	20.3022	1
7	-5	5		10.2092	9.5568	1	10	-1	3		15.6146	16.7672	1
7	-5	1		10.1049	6.3736	1	10	-1	1		18.6007	18.3814	1
7	-6	4		19.1833	17.8674	1	10	0	4		11.0497	11.5405	1
7	-6	6		10.2074	8.6540	1	10	0	2		23.9756	24.1477	1
7	-8	2		14.8407	14.0142	1	10	0	1		9.1313	17.0036	1
7	-8	4		21.6581	21.0836	1	11	-3	1		8.8050	11.1421	1
7	-8	6		11.2274	12.7971	1	11	-7	1		8.8178	6.3225	1
7	-11	3		14.4470	14.2126	1	11	-8	0		14.1805	15.1245	1
7	-11	1		24.5865	23.8144	1	12	-3	1		20.2202	21.4302	1
7	-13	2		8.3646	13.0032	1	0	-17	-1		9.2651	8.6732	1
8	-12	2		18.1793	20.2188	1	0	-16	-2		14.0212	14.7387	1
8	-10	2		19.3009	17.5121	1	0	-16	-4		20.6694	22.2197	1
8	-9	1		30.0267	29.6315	1	0	-15	-5		24.1581	22.9606	1
8	-9	3		28.7857	28.8753	1	0	-15	-3		41.6001	41.3622	1
8	-8	4		11.1349	12.2554	1	0	-15	-1		39.1100	38.2688	1
8	-7	3		10.7532	9.8484	1	0	-14	-4		9.6499	5.9993	1
8	-7	5		14.9259	13.5679	1	0	-13	-7		18.5163	20.1936	1
8	-6	4		22.9095	23.5993	1	0	-13	-5		18.2889	17.5510	1
8	-6	2		35.7717	36.3943	1	0	-13	-3		30.2047	30.2162	1
8	-6	1		8.3360	18.5255	1	0	-13	-1		22.4415	23.4103	1
8	-5	5		9.3151	8.5310	1	0	-12	-2		47.7293	47.1044	1
8	-4	3		8.9259	12.8913	1	0	-12	-4		56.7348	55.3406	1
8	-3	1		43.9631	44.1379	1	0	-12	-6		49.4939	47.9686	1
8	-3	3		41.0321	40.1336	1	0	-12	-8		30.1694	28.9481	1

PZ <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*	PZ <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*
0	-11	-1		9.4086	8.1087	1	1	-6	-6		20.4703	21.4784	1
0	-10	-2		29.1982	29.5563	1	1	-6	-4		25.8557	25.4953	1
0	-10	-4		13.2191	13.8172	1	1	-6	-2		36.4844	36.9404	1
0	-10	-8		20.7360	21.2704	1	1	-6	0		14.0005	13.2461	1
0	-9	-9		36.0314	37.0410	1	1	-7	-3		10.0126	10.2551	1
0	-9	-7		41.7563	40.8116	1	1	-7	-10		9.8604	4.6337	1
0	-9	-5		52.1465	53.1984	1	1	-8	-10		9.3952	7.3743	1
0	-9	-3		48.5824	48.6517	1	1	-8	-6		20.1778	19.4817	1
0	-9	-1		78.8270	82.4728	1	1	-8	-4		30.0279	30.3134	1
0	-8	-1		13.2140	5.1696	1	1	-8	-2		33.7174	31.8972	1
0	-8	-4		9.4924	7.0196	1	1	-8	0		14.9959	15.7725	1
0	-8	-5		7.3081	5.0835	1	1	-9	-1		20.2383	20.5717	1
0	-8	-6		15.3789	13.3719	1	1	-9	-3		8.3321	4.0268	1
0	-8	-10		11.5900	8.6514	1	1	-9	-5		7.8325	6.6591	1
0	-7	-7		11.8370	10.8674	1	1	-9	-7		14.8378	14.4245	1
0	-7	-5		37.7042	37.8909	1	1	-9	-9		8.3987	5.4780	1
0	-7	-1		8.5382	10.1533	1	1	-10	-4		15.0482	15.5739	1
0	-6	-2		103.8391	104.2044	1	1	-10	0		10.5114	13.9286	1
0	-6	-4		78.2872	77.8149	1	1	-11	-1		15.9776	16.7706	1
0	-6	-5		6.8158	4.7732	1	1	-11	-3		22.9239	24.0506	1
0	-6	-6		55.3660	54.7842	1	1	-11	-5		13.7842	15.7140	1
0	-6	-8		56.2490	56.2501	1	1	-11	-7		19.5433	18.0478	1
0	-6	-10		34.3514	32.9641	1	1	-11	-9		27.1943	26.6491	1
0	-5	-7		9.6892	8.1753	1	1	-12	-5		8.0213	5.3937	1
0	-5	-5		14.0174	14.4456	1	1	-12	-4		15.6373	15.0699	1
0	-5	-3		29.8191	27.6339	1	1	-12	-1		9.0222	8.5280	1
0	-4	-6		7.6742	7.1759	1	1	-13	-1		13.0151	14.3138	1
0	-4	-8		14.5544	14.7078	1	1	-13	-7		15.7437	13.4155	1
0	-4	-10		10.8444	13.0085	1	1	-14	-6		16.6797	17.6080	1
0	-3	-11		34.4759	34.5445	1	1	-14	-4		16.5893	17.6820	1
0	-3	-9		48.1796	49.7496	1	1	-14	-2		21.3904	21.1857	1
0	-3	-7		71.9950	72.8118	1	1	-14	0		19.1558	19.4686	1
0	-3	-5		103.3852	101.2723	1	1	-15	-1		11.4172	12.9089	1
0	-3	-3		147.1741	144.7526	1	1	-15	-3		19.6138	17.9236	1
0	-2	-4		31.9121	30.6577	1	1	-15	-5		16.1251	14.0763	1
0	-2	-6		26.6736	25.7961	1	1	-16	-4		16.0478	14.0813	1
0	-1	-9		17.7367	17.2903	1	1	-16	-2		17.7842	16.2488	1
0	-1	-7		18.2934	16.8432	1	1	-16	0		11.8455	11.4756	1
0	0	-4		113.3399	107.9415	1	1	-17	-1		15.6546	17.4242	1
0	0	-6		93.3286	92.8668	1	1	-17	-2		8.9462	8.8023	1
0	0	-7		8.8365	10.3665	1	2	-17	-1		27.3047	25.5543	1
0	0	-8		61.9819	60.9105	1	2	-16	0		13.5414	13.5848	1
0	0	-10		64.7885	63.5269	1	2	-16	-4		16.7733	13.5029	1
1	-1	-5		24.4101	22.3740	1	2	-14	0		39.2656	38.5120	1
1	-2	-10		14.2492	8.2608	1	2	-14	-2		35.2670	35.1679	1
1	-2	-8		14.2623	12.8362	1	2	-14	-4		42.7183	41.3473	1
1	-2	-6		11.2471	11.2624	1	2	-14	-6		22.5385	21.4713	1
1	-2	-4		7.7570	8.0255	1	2	-13	-7		18.4487	17.9161	1
1	-3	-7		7.7640	9.1147	1	2	-13	-3		14.9462	15.0576	1
1	-3	-9		23.0731	24.0217	1	2	-13	-1		16.0816	18.9499	1
1	-4	-10		8.4478	7.2647	1	2	-12	0		8.3848	10.2315	1
1	-4	-6		23.8031	24.4984	1	2	-12	-2		20.2753	20.5547	1
1	-4	-4		23.5220	22.6938	1	2	-12	-4		10.4480	11.7123	1
1	-5	-3		18.4344	17.4079	1	2	-12	-6		9.1215	6.4447	1
1	-5	-7		16.8127	15.3261	1	2	-12	-7		8.1362	1.2896	1
1	-6	-8		8.3573	3.7136	1							

P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*
2	-11	-9		31.4165	32.3753	1	2	-1	-7		55.4100	55.1488	1
2	-11	-7		41.1129	40.1844	1	2	-1	-5		43.5576	42.3787	1
2	-11	-5		45.9176	46.2682	1	2	0	-6		46.6019	46.0894	1
2	-11	-4		8.0193	11.3352	1	2	0	-8		36.8420	35.5926	1
2	-11	-3		45.9787	45.7023	1	3	-1	-11		15.6673	13.9215	1
2	-11	-1		46.6042	48.1691	1	3	-2	-6		16.0920	17.1688	1
2	-10	0		28.2908	29.0001	1	3	-3	-3		8.3067	10.0347	1
2	-10	-2		45.2335	45.9229	1	3	-3	-5		46.5193	46.8054	1
2	-10	-4		26.6765	27.1325	1	3	-3	-7		14.9452	14.5728	1
2	-10	-6		19.3978	20.2524	1	3	-4	-10		11.3539	8.1391	1
2	-10	-8		17.0103	18.5056	1	3	-4	-8		17.2344	18.5491	1
2	-10	-9		9.3504	8.6249	1	3	-4	-6		9.0616	9.2767	1
2	-10	-10		16.6752	16.1971	1	3	-4	-4		15.0032	15.6615	1
2	-9	-7		18.8108	19.7029	1	3	-4	-2		19.6771	19.2296	1
2	-9	-3		7.1435	5.1575	1	3	-4	0		30.3167	28.6941	1
2	-9	-1		7.8389	8.3188	1	3	-5	-1		7.3578	7.7762	1
2	-8	0		72.4628	71.7316	1	3	-5	-3		22.9989	22.6281	1
2	-8	-2		85.4334	86.1026	1	3	-5	-7		14.4198	13.8037	1
2	-8	-4		54.0416	54.2468	1	3	-5	-8		7.8479	4.8347	1
2	-8	-6		62.0316	63.6819	1	3	-6	-11		10.2281	13.8759	1
2	-8	-8		54.7727	53.5436	1	3	-6	-10		8.3163	12.5283	1
2	-8	-9		8.7110	13.7905	1	3	-6	-8		11.5346	14.5554	1
2	-8	-10		28.2473	27.5920	1	3	-6	-4		6.9533	9.5687	1
2	-7	-11		19.5875	18.5797	1	3	-6	-2		43.5322	44.3622	1
2	-7	-9		37.7914	36.6564	1	3	-6	0		22.3001	21.9036	1
2	-7	-7		36.2673	35.3627	1	3	-7	-3		7.1860	4.0969	1
2	-7	-5		55.9077	57.0428	1	3	-8	-10		16.5234	16.0069	1
2	-7	-3		35.7843	35.9959	1	3	-8	-8		13.0640	14.9837	1
2	-7	-1		32.7161	32.5362	1	3	-8	-4		14.9808	16.2927	1
2	-6	0		17.8687	17.5380	1	3	-8	-2		35.6489	36.5000	1
2	-6	-4		21.5932	21.8854	1	3	-8	0		32.0146	31.4702	1
2	-6	-5		6.3795	2.2055	1	3	-9	-1		7.9967	4.3689	1
2	-6	-10		11.4100	9.8851	1	3	-9	-3		8.9727	12.6684	1
2	-5	-11		39.1430	38.8517	1	3	-9	-5		8.2514	8.1777	1
2	-5	-9		44.3404	43.5752	1	3	-9	-7		11.0316	12.9882	1
2	-5	-7		40.1044	39.6325	1	3	-10	-8		8.9444	10.0174	1
2	-5	-5		76.9162	77.4995	1	3	-10	-5		7.4271	5.6854	1
2	-5	-3		113.8863	112.4570	1	3	-10	-3		8.2827	11.4999	1
2	-5	-1		115.7512	112.7588	1	3	-10	-2		7.2853	7.4892	1
2	-4	-4		69.0075	67.5961	1	3	-10	-1		8.2067	13.6237	1
2	-4	-6		42.9395	43.1900	1	3	-10	0		13.9919	13.0777	1
2	-4	-8		32.0950	32.6006	1	3	-11	-1		19.1681	19.5690	1
2	-4	-10		30.4669	30.1438	1	3	-11	-2		9.0490	6.8738	1
2	-4	-12		28.4944	26.4121	1	3	-11	-3		12.9397	14.4332	1
2	-3	-11		10.0717	11.1359	1	3	-11	-5		39.8287	39.0477	1
2	-3	-9		8.0137	10.5180	1	3	-11	-7		22.3673	21.5400	1
2	-3	-8		8.4692	5.6379	1	3	-12	-5		10.5522	5.4518	1
2	-3	-5		25.6996	25.7616	1	3	-12	-4		9.4705	7.9038	1
2	-2	-4		86.8267	83.8099	1	3	-12	0		14.6970	14.5316	1
2	-2	-6		68.5332	66.7394	1	3	-13	-3		8.3446	6.4370	1
2	-2	-8		50.9357	49.2310	1	3	-13	-6		9.9640	12.4967	1
2	-2	-10		38.9765	38.4711	1	3	-13	-7		11.6887	9.4652	1
2	-1	-11		15.4934	16.4379	1	3	-14	-6		12.4735	13.8203	1
2	-1	-9		27.2099	26.6566	1	3	-14	-4		17.2706	17.7433	1
2	-1	-9		29.1371	27.9942	1	3	-14	-2		24.7949	24.4078	1

P2 <sub>1</sub>	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*	P2 <sub>1</sub>	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*
3	-14	0		19.3691	19.3658	1	4	-5	-7		11.2087	8.6388	1
3	-15	-1		15.7994	16.5760	1	4	-5	-3		8.7914	10.5680	1
3	-15	-3		8.7452	11.6126	1	4	-5	-1		34.7753	34.5132	1
3	-16	-4		11.1025	6.6362	1	4	-4	-2		16.6462	15.9327	1
3	-16	-3		8.5829	12.1043	1	4	-4	-4		23.7219	24.1412	1
3	-16	-2		16.1265	15.4142	1	4	-4	-6		20.7750	19.4237	1
3	-16	0		11.5315	10.8956	1	4	-4	-8		9.9926	7.0850	1
4	-16	0		19.2112	19.3640	1	4	-4	-12		13.9165	9.2761	1
4	-16	-2		17.3094	18.1525	1	4	-3	-11		45.9591	45.1077	1
4	-16	-4		18.8723	17.7948	1	4	-3	-9		57.2689	56.0344	1
4	-15	-5		35.8371	34.0252	1	4	-3	-7		72.0344	71.1782	1
4	-15	-3		28.8351	27.6982	1	4	-3	-5		75.2755	76.9624	1
4	-15	-1		37.2842	36.5160	1	4	-3	-3		92.0632	90.9992	1
4	-14	-4		15.5326	15.2361	1	4	-3	-1		138.3279	133.5967	1
4	-14	-5		9.2395	8.0565	1	4	-2	0		26.7474	25.2140	1
4	-13	-7		21.6699	21.5856	1	4	-2	-2		16.5177	15.3525	1
4	-13	-5		23.2004	22.5640	1	4	-2	-4		6.9282	5.7928	1
4	-13	-3		15.3044	18.7413	1	4	-2	-6		11.8412	13.1536	1
4	-13	-1		28.8504	29.3071	1	4	-2	-8		18.0052	16.6034	1
4	-12	0		53.8995	52.8830	1	4	-2	-9		8.4704	9.4752	1
4	-12	-2		44.8810	45.3874	1	4	-2	-10		14.6912	14.2841	1
4	-12	-4		35.4971	35.9133	1	4	-1	-11		13.5968	14.2958	1
4	-12	-6		30.1329	30.6644	1	4	-1	-7		22.1642	21.2725	1
4	-12	-8		37.0220	37.3206	1	4	-1	-5		29.2372	28.9622	1
4	-11	-7		8.2665	6.1151	1	4	-1	-3		9.3043	7.8008	1
4	-10	0		14.0111	14.8614	1	4	0	0		86.8787	83.9100	1
4	-10	-2		18.6177	19.8018	1	4	0	-4		161.4089	161.2207	1
4	-10	-4		22.7903	23.2093	1	4	0	-6		85.3845	83.9860	1
4	-10	-6		26.3189	26.9323	1	4	0	-8		69.3484	67.9668	1
4	-10	-8		9.6622	9.1550	1	4	0	-10		46.1571	44.9749	1
4	-10	-10		9.0932	7.4111	1	4	0	-12		34.0344	32.4402	1
4	-9	-11		22.1986	19.8165	1	5	-1	-1		13.0575	14.5593	1
4	-9	-9		35.3775	34.4032	1	5	-1	-2		5.9569	14.4101	1
4	-9	-7		35.1993	37.2322	1	5	-1	-3		17.2508	17.2603	1
4	-9	-5		54.7596	55.0176	1	5	-1	-5		10.1413	12.2060	1
4	-9	-3		66.6660	67.7049	1	5	-1	-7		17.0322	18.2608	1
4	-9	-1		38.4313	39.4785	1	5	-2	-12		10.1566	10.3680	1
4	-8	-2		11.1417	12.4292	1	5	-2	-10		11.9469	11.7465	1
4	-8	-4		25.0455	27.6910	1							
4	-8	-6		8.9125	5.4976	1	5	-2	-8		9.1960	8.4102	1
4	-8	-8		12.4050	10.9078	1	5	-2	-4		10.6079	11.6776	1
4	-8	-6		8.7103	5.4976	1	5	-2	-2		18.5014	19.5733	1
4	-7	-9		26.3650	26.4929	1	5	-2	0		15.3693	14.3698	1
4	-7	-5		7.3312	4.4100	1	5	-3	-1		37.0221	35.9574	1
4	-7	-3		17.6600	18.4943	1	5	-3	-3		33.9971	34.4702	1
4	-7	-1		9.2694	10.1409	1	5	-3	-5		11.8254	13.2838	1
4	-6	0		82.6625	82.7759	1	5	-3	-7		16.2347	19.1727	1
4	-6	-2		75.6054	76.1353	1	5	-3	-9		8.5650	8.1106	1
4	-6	-4		54.7547	56.6799	1	5	-4	-8		8.6601	9.5238	1
4	-6	-6		65.1962	67.2003	1	5	-4	-7		8.5962	9.9859	1
4	-6	-8		42.3949	42.5306	1	5	-4	-5		5.7683	11.8239	1
4	-6	-10		36.8450	36.3564	1	5	-4	-4		37.5369	38.7695	1
4	-6	-11		11.0408	13.5925	1	5	-5	-1		10.4297	12.4320	1
4	-6	-12		33.1122	32.8784	1	5	-5	-3		8.0352	9.6179	1
4	-5	-11		10.3998	7.7841	1	5	-5	-5		7.6764	12.9495	1

P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*	P2 <sub>1</sub>	h	k	l	F(obs)	F(calc)	SF*
5	-5	-7		15.0287	15.1033	1	6	-9	-3		9.4533	4.0053	1
5	-5	-11		8.8348	3.9466	1	6	-9	-2		7.5864	3.2257	1
5	-6	-10		16.9491	17.5834	1	6	-9	-1		12.7498	12.0855	1
5	-6	-8		18.3693	20.7426	1	6	-8	0		62.8642	63.2912	1
5	-6	-6		13.8308	15.4310	1	6	-8	-1		7.0985	17.3177	1
5	-6	-4		10.6513	12.9712	1	6	-8	-2		48.0875	49.6422	1
5	-6	0		28.5922	28.2668	1	6	-8	-4		54.8839	56.0795	1
5	-8	-10		11.8153	11.6602	1	6	-8	-6		47.1448	48.6382	1
5	-8	-8		15.1044	17.0624	1	6	-8	-7		9.0287	19.3884	1
5	-8	-6		8.3847	13.1894	1	6	-8	-8		28.8329	28.3473	1
5	-8	0		21.0169	22.1726	1	6	-8	-10		37.5168	38.3045	1
5	-9	-1		8.4725	7.9136	1	6	-7	-11		22.2735	18.8734	1
5	-9	-3		17.5206	18.7244	1	6	-7	-9		24.8426	23.3213	1
5	-9	-5		17.3974	18.1537	1	6	-7	-7		22.6460	22.8982	1
5	-9	-11		11.9926	10.8437	1	6	-7	-5		16.0901	18.2466	1
5	-10	-4		12.6104	14.7873	1	6	-7	-3		53.3316	55.2659	1
5	-10	-2		9.2258	3.7210	1	6	-7	-2		7.1917	18.8298	1
5	-10	-1		8.8390	2.2996	1	6	-7	-1		42.1963	43.4397	1
5	-11	-1		24.9795	25.7090	1	6	-6	-1		8.1139	8.0173	1
5	-11	-3		25.1188	26.1599	1	6	-6	-2		13.6949	14.5547	1
5	-11	-5		12.0304	14.4213	1	6	-6	-8		12.7864	11.1297	1
5	-11	-7		13.5141	15.6860	1	6	-6	-10		10.7314	3.9054	1
5	-12	-6		12.3902	12.2870	1	6	-5	-11		22.4481	21.0253	1
5	-12	-2		18.8454	18.9518	1	6	-5	-9		41.9494	40.5521	1
5	-13	-3		14.6273	14.2976	1	6	-5	-7		59.8697	60.5052	1
5	-13	-4		9.0432	4.9015	1	6	-5	-5		52.0865	53.8636	1
5	-13	-5		10.5057	12.1833	1	6	-5	-3		54.0470	55.3048	1
5	-14	-6		11.0234	11.4655	1	6	-5	-1		48.0087	48.4437	1
5	-14	0		13.2036	14.8247	1	6	-4	0		40.6717	41.4301	1
5	-15	0		8.7462	10.3104	1	6	-4	-2		33.3253	34.6280	1
5	-15	-1		9.8564	11.4567	1	6	-4	-4		38.3097	39.6545	1
5	-16	-2		11.6021	6.3448	1	6	-4	-6		42.2176	42.9565	1
6	-15	-3		11.4885	11.5863	1	6	-4	-8		33.1815	33.2133	1
6	-14	0		17.0980	16.6491	1	6	-4	-10		24.7851	22.4019	1
6	-14	-2		22.8904	22.7397	1	6	-4	-12		16.9324	14.8150	1
6	-14	-4		20.7157	21.6664	1	6	-3	-9		11.0892	11.8710	1
6	-14	-6		24.5358	25.4201	1	6	-3	-7		22.7012	23.9668	1
6	-13	-5		13.6717	13.8579	1	6	-3	-5		15.8660	16.0714	1
6	-13	-3		8.2456	8.8241	1	6	-3	-3		13.4844	14.1332	1
6	-13	-1		11.7884	12.3741	1	6	-3	-1		6.9022	10.3702	1
6	-12	0		9.6080	5.7110	1	6	-2	-2		80.8892	81.6842	1
6	-12	-6		9.8450	11.5176	1	6	-2	0		43.7704	44.3198	1
6	-12	-7		13.9510	4.7945	1	6	-2	-6		27.5978	29.1184	1
6	-11	-9		26.4300	26.7293	1	6	-2	-4		52.0382	54.2204	1
6	-11	-7		29.9309	28.4048	1	6	-2	-8		35.2090	36.7188	1
6	-11	-5		31.1504	32.1234	1	6	-2	-10		28.2150	28.0539	1
6	-11	-3		40.2961	41.2491	1	6	-2	-12		30.0810	28.9563	1
6	-11	-1		40.3438	40.9388	1	6	-1	-11		27.6456	26.9231	1
6	-10	0		23.4796	23.0753	1	6	-1	-10		9.1296	14.2714	1
6	-10	-4		19.0127	19.0428	1	6	-1	-9		26.9188	26.3915	1
6	-10	-6		24.5261	26.4355	1	6	-1	-7		30.9011	31.6478	1
6	-10	-8		17.0538	17.0062	1	6	-1	-5		55.6372	56.8651	1
6	-10	-10		14.2805	13.5806	1	6	-1	-3		27.1056	27.8156	1
6	-9	-7		9.5052	10.2700	1	6	-1	-1		44.6796	44.6418	1
6	-9	-5		9.3812	8.5712	1	6	0	0		49.1096	49.5379	1

P2 <sub>1</sub>	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*	P2 <sub>1</sub>	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*
6	0	-2		33.1200	34.2818	1	8	-13	-1		14.6859	14.0722	1
6	0	-4		35.4807	37.2980	1	8	-12	0		19.9659	18.9343	1
6	0	-6		16.0412	18.5300	1	8	-12	-2		30.6180	19.7100	1
6	0	-10		19.5964	22.1060	1	8	-12	-4		33.0573	32.5480	1
6	0	-12		12.5546	12.8848	1	8	-12	-6		28.4748	27.9482	1
7	-1	-1		18.8765	19.7303	1	8	-12	-8		15.5859	16.6057	1
7	-1	-5		9.9449	10.8056	1	8	-11	-3		9.8113	7.9352	1
7	-1	-11		9.7517	12.3643	1	8	-10	0		16.9946	19.0174	1
7	-2	-6		20.9307	20.8974	1	8	-10	-2		10.8931	10.0451	1
7	-3	-1		9.7161	14.3588	1	8	-10	-4		8.9075	12.0051	1
7	-3	-3		25.7565	27.8812	1	8	-10	-8		17.6836	15.5688	1
7	-3	-7		7.6631	11.9592	1	8	-9	-9		24.2341	24.0018	1
7	-3	-9		20.6987	21.8816	1	8	-9	-7		32.2093	33.8048	1
7	-4	-11		9.3839	11.7891	1	8	-9	-5		17.1970	19.3275	1
7	-4	-8		9.2918	7.8293	1	8	-9	-3		23.5153	24.6048	1
7	-4	-4		15.4392	15.0568	1	8	-9	-2		8.1814	20.5432	1
7	-4	-2		10.7946	10.5228	1	8	-9	-1		39.1183	40.3198	1
7	-4	0		19.2947	21.2587	1	8	-8	0		11.9835	12.5399	1
7	-5	-1		15.6691	16.9184	1	8	-8	-2		18.6807	18.9471	1
7	-5	-3		8.1861	10.9842	1	8	-8	-6		10.1223	13.6258	1
7	-5	-11		10.6063	10.2771	1	8	-8	-8		10.7026	12.9800	1
7	-6	-9		9.1328	16.3051	1	8	-7	-7		14.4224	15.0738	1
7	-6	-6		25.0800	27.7376	1	8	-7	-5		14.2562	12.6700	1
7	-8	-4		11.2143	18.1191	1	8	-7	-3		14.0158	14.0787	1
7	-6	0		8.6759	7.9364	1	8	-7	-1		10.4112	10.1741	1
7	-7	-3		7.4584	3.9346	1	8	-6	0		38.2469	38.3536	1
7	-8	-8		11.3811	10.9137	1	8	-6	-2		30.7134	32.8833	1
7	-8	-7		8.5697	12.3664	1	8	-6	-3		8.6442	24.8751	1
7	-8	-6		24.5989	22.6966	1	8	-6	-4		46.1611	46.9737	1
7	-8	-4		16.0701	18.1191	1	8	-6	-6		30.5626	31.7971	1
7	-8	-2		11.4570	10.5474	1	8	-6	-8		26.6463	27.8758	1
7	-9	-1		15.0479	16.1747	1	8	-6	-10		28.5152	29.0855	1
7	-10	-10		8.9523	9.5309	1	8	-5	-5		18.7394	21.5960	1
7	-10	-9		9.5896	4.5843	1	8	-5	-3		14.7830	17.7194	1
7	-10	-2		12.3678	11.3127	1	8	-4	0		14.2605	15.0467	1
7	-10	-1		8.3900	18.7179	1	8	-4	-1		7.8691	15.8986	1
7	-10	0		17.5548	16.1884	1	8	-4	-6		10.6766	7.4644	1
7	-11	-1		21.4301	20.1120	1	8	-4	-8		12.8251	12.7947	1
7	-11	-3		27.9740	26.5900	1	8	-4	-10		12.2532	11.7061	1
7	-11	-5		11.9848	9.6946	1	8	-4	-12		9.1555	4.9691	1
7	-11	-9		20.6066	22.5019	1	8	-3	-11		27.1871	27.1085	1
7	-12	-3		9.0557	8.9532	1	8	-3	-9		32.6504	32.7434	1
7	-13	-1		11.0390	10.5664	1	8	-3	-7		39.3486	40.2145	1
7	-13	-2		8.7617	12.8789	1	8	-3	-5		59.8168	60.4853	1
7	-13	-5		9.9086	7.8045	1	8	-3	-3		59.0116	60.4527	1
7	-14	-6		19.0653	17.7036	1	8	-3	-1		45.3751	45.0363	1
7	-14	-4		14.5253	15.0293	1	8	-2	0		8.2035	9.2793	1
7	-14	-3		9.4184	14.1914	1	8	-2	-2		12.0360	13.4979	1
7	-14	-2		16.2892	13.2580	1	8	-2	-3		7.6870	19.9186	1
7	-14	0		18.1224	15.1704	1	8	-2	-5		7.1019	24.6360	1
8	-14	-4		10.2954	12.7933	1	8	-2	-6		13.6398	14.9826	1
8	-13	-5		21.6919	20.0230	1	8	-2	-7		8.5141	12.4220	1
8	-13	-4		8.5812	7.7948	1	8	-2	-12		10.2310	10.6614	1
8	-13	-3		14.3834	17.8566	1	8	-1	-12		8.5413	13.0783	1
8	-13	-2		9.6545	8.4498	1	8	-1	-9		17.9207	17.0872	1

P2 <sub>1</sub>	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*	P2 <sub>1</sub>	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*
8	-1	-5		14.8464	15.6486	1	10	-10	-2		14.4884	16.2973	1
8	-1	-3		10.4073	13.2015	1	10	-10	-4		10.1982	12.2292	1
8	0	0		66.4231	67.6626	1	10	-10	-7		9.6787	20.1423	1
8	0	-2		71.5352	72.3432	1	10	-8	0		20.4563	20.8142	1
8	0	-4		36.8484	36.4761	1	10	-8	-2		26.7599	27.5623	1
8	0	-6		54.3929	55.0147	1	10	-8	-4		32.1351	33.0326	1
8	0	-8		58.1385	55.9160	1	10	-8	-6		25.0013	24.3582	1
8	0	-10		39.2547	37.1670	1	10	-8	-8		31.1365	31.5102	1
8	0	-12		33.4242	32.4844	1	10	-7	-10		9.1956	17.5215	1
9	-1	-3		7.6721	8.9382	1	10	-7	-7		24.2182	24.5860	1
9	-1	-7		12.2516	15.3949	1	10	-7	-5		23.9353	24.4044	1
9	-1	-9		9.0893	12.7942	1	10	-7	-1		16.8962	15.9567	1
9	-2	-12		10.0526	11.0299	1	10	-6	-8		8.9003	3.2509	1
9	-2	-8		9.5732	12.1771	1	10	-6	-10		9.9811	2.8923	1
9	-2	-4		12.4360	12.0865	1	10	-5	-11		27.2326	28.1828	1
9	-2	-2		18.6431	18.9000	1	10	-5	-9		20.4137	21.5086	1
9	-3	-1		12.4155	13.9007	1	10	-5	-7		21.0995	21.6224	1
9	-3	-4		8.5647	16.6942	1	10	-5	-5		26.7790	27.8599	1
9	-3	-5		19.7592	21.3732	1	10	-5	-3		32.9965	33.3677	1
9	-3	-7		12.5819	16.8782	1	10	-5	-1		39.8021	40.0456	1
9	-3	-9		12.7213	17.5153	1	10	-4	0		18.8677	21.5020	1
9	-4	-8		17.6113	16.0013	1	10	-4	-2		22.9358	24.9643	1
9	-4	-7		8.3343	9.4180	1	10	-4	-4		21.7506	21.3083	1
9	-5	-2		8.3166	10.5876	1	10	-4	-6		12.6229	15.2861	1
9	-5	-3		8.3569	9.1201	1	10	-4	-7		8.1558	20.3495	1
9	-5	-4		9.1520	12.7869	1	10	-4	-8		14.7086	14.1485	1
9	-5	-5		14.7929	16.0368	1	10	-4	-10		14.1520	16.2942	1
9	-5	-9		8.8435	8.5419	1	10	-3	-11		14.1329	10.6529	1
9	-5	-11		12.2732	12.7911	1	10	-3	-5		9.6382	7.8678	1
9	-6	-6		9.4751	13.1896	1	10	-3	-3		12.8386	12.2692	1
9	-6	-4		19.8468	20.8266	1	10	-3	-2		9.1414	14.3271	1
9	-6	-2		25.3910	26.0436	1	10	-3	-1		17.9567	17.3950	1
9	-7	-6		8.1249	7.1738	1	10	-2	0		24.0425	23.2123	1
9	-7	-7		10.5350	5.9966	1	10	-2	-2		13.9799	15.5993	1
9	-7	-8		10.8309	9.3733	1	10	-2	-4		18.3540	20.9057	1
9	-8	-8		8.0980	8.6026	1	10	-2	-6		34.7814	36.2979	1
9	-8	-4		8.8975	12.8952	1	10	-2	-8		19.8502	22.2683	1
9	-8	-2		8.5606	14.0061	1	10	-2	-9		8.3651	22.7200	1
9	-8	-1		8.0136	10.1843	1	10	-2	-10		15.8664	14.5238	1
9	-9	-1		9.3599	10.4104	1	10	-1	-9		17.1375	21.7559	1
9	-9	-3		10.9979	11.0438	1	10	-7	-7		14.4448	24.5860	1
9	-9	-7		17.7870	17.1470	1	10	-1	-5		16.0756	15.5213	1
9	-10	-8		12.0139	11.8103	1	10	-1	-4		8.6070	18.9719	1
9	-10	-3		9.6097	10.1634	1	10	-1	-3		27.5910	29.6805	1
9	-11	-5		8.4788	12.1420	1	10	-1	-1		14.9523	15.7482	1
9	-12	-6		11.9038	13.2012	1	10	0	-2		10.4239	6.3601	1
9	-12	-5		11.0498	8.1528	1	10	0	-4		21.6916	19.4305	1
9	-12	-4		11.7631	12.2899	1	10	0	-6		16.1682	14.7147	1
9	-12	-1		8.3026	11.1266	1	10	0	-8		22.9100	22.1980	1
9	-12	0		11.5050	13.0699	1	11	-1	-5		15.7576	15.9747	1
9	-13	-4		7.7194	3.7466	1	11	-2	-11		9.9594	13.0332	1
10	-11	-7		20.1775	22.4314	1	11	-2	-10		10.1500	14.5481	1
10	-11	-5		21.2896	23.7928	1	11	-2	-8		9.2140	9.4842	1
10	-11	-3		16.6372	17.7571	1	11	-2	-4		10.5574	11.7982	1
10	-11	-1		16.2556	17.6757	1	11	-2	0		10.6985	9.2230	1



P2 <sub>1</sub>	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*	P2 <sub>1</sub>	h	k	l	F <sub>(obs)</sub>	F <sub>(calc)</sub>	SF*
11	-3	-1		10.8261	13.8168	1	13	-4	-2		9.9188	5.7563	1
11	-3	-7		17.8154	20.2700	1	13	-5	-3		10.2731	10.2309	1
11	-4	-2		13.7597	12.6041	1	13	-5	-7		9.1149	11.8397	1
11	-4	0		9.7092	8.7613	1	13	-6	-6		14.7173	19.0449	1
11	-5	-1		10.2220	12.5518	1	13	-6	-4		8.9127	11.4421	1
11	-5	-7		8.4473	11.0359	1	0	-5	-1		17.7843	18.7938	2
11	-5	-9		9.1768	8.8537	1	0	-5	1		18.0505	18.7938	2
11	-6	-2		10.2097	12.3578	1	0	-4	2		29.6186	28.6048	2
11	-6	-10		13.3464	18.0821	1	0	-4	1		4.6154	3.8542	2
11	-7	-5		8.4380	10.2877	1	0	-4	0		41.2358	40.3506	2
11	-7	-7		10.0056	7.4671	1	0	-4	-2		29.0696	28.6046	2
11	-8	-5		9.6130	8.8601	1	0	-3	-1		129.3514	132.6897	2
11	-8	-2		12.8205	11.6030	1	0	-3	1		124.3630	132.6895	2
11	-9	-1		8.7494	10.3298	1	0	-2	3		6.5094	6.5871	2
11	-9	-5		11.0274	12.6483	1	0	-2	2		12.4125	9.8587	2
11	-10	-6		13.8778	11.0991	1	0	-2	0		15.0461	13.8627	2
11	-10	-4		18.8680	16.8943	1	0	-2	-2		12.2601	9.8587	2
11	-10	-3		9.2532	11.9744	1	0	-1	-3		62.7076	59.7593	2
12	-8	-4		11.4252	15.0689	1	0	-1	-1		40.2405	37.4609	2
12	-8	-6		13.3116	13.3594	1	0	-1	1		39.5992	37.4607	2
12	-6	-2		17.3887	17.5075	1	0	-1	3		62.9083	59.7593	2
12	-6	-4		12.0238	11.6616	1	0	0	2		182.1537	171.8317	2
12	-6	-6		11.8525	12.2838	1	0	0	1		13.7993	8.3286	2
12	-6	-7		11.3296	16.1848	1	1	-1	3		6.6611	6.2172	2
12	-6	-8		17.6980	16.8206	1	1	-1	2		4.6287	5.4709	2
12	-5	-9		12.3897	13.7599	1	1	-1	1		14.3401	10.4294	2
12	-5	-7		9.8409	13.8873	1	1	-1	0		8.5502	8.1724	2
12	-5	-5		12.0699	8.5470	1	1	-1	-3		71.5145	67.8131	2
12	-4	-4		10.7426	11.3451	1	1	-2	-2		18.4207	17.1176	2
12	-4	-8		9.0947	8.1870	1	1	-2	-1		5.8550	9.3327	2
12	-3	-9		24.1696	21.6696	1	1	-2	0		4.8035	3.5582	2
12	-3	-8		8.4588	19.0706	1	1	-2	2		48.4979	47.5427	2
12	-3	-7		24.3617	22.9082	1	1	-3	1		75.9466	82.8260	2
12	-3	-5		13.7765	14.9912	1	1	-3	-1		7.1023	5.3221	2
12	-3	-3		17.1131	18.2313	1	1	-4	-2		17.7039	18.4972	2
12	-3	-2		8.7788	18.4694	1	1	-4	0		74.5984	70.8816	2
12	-3	-1		22.1059	22.6329	1	1	-5	-1		36.5602	36.4267	2
12	-2	-2		10.1682	8.3281	1	2	-4	0		83.0945	81.9670	2
12	-2	-7		9.4818	19.4245	1	2	-4	-2		99.2011	99.0520	2
12	-1	-4		9.6461	17.2598	1	2	-3	-3		47.5672	48.1073	2
12	-1	-3		8.9104	12.6510	1	2	-3	-1		44.8860	44.3882	2
12	0	0		24.2184	22.0068	1	2	-3	1		29.9932	30.0716	2
12	0	-2		20.9310	21.7363	1	2	-2	2		102.9606	117.9071	2
12	0	-4		37.6412	36.7369	1	2	-2	0		115.2608	111.3414	2
12	0	-6		30.1920	28.4479	1	2	-2	-2		29.4287	34.6987	2
12	0	-8		11.0931	10.2658	1	2	-1	-3		89.7533	88.9101	2
12	0	-10		19.6623	18.3199	1	2	-1	-1		125.3352	129.8605	2
13	-1	-5		9.8562	7.7727	1	2	-1	1		35.3105	38.3665	2
13	-1	-8		9.8292	6.5246	1	2	0	2		66.5389	66.2798	2
13	-2	-8		10.3977	9.9901	1	2	0	0		37.9862	36.6680	2
13	-2	-6		15.1231	15.2521	1	2	0	-1		5.0663	9.0292	2
13	-3	-3		16.6591	20.4508	1	3	-1	1		32.3623	30.6844	2
13	-3	-8		9.2985	10.7037	1	3	-1	-1		66.2585	63.5272	2
13	-4	-8		10.3980	12.6883	1	3	-1	-3		13.1628	12.8891	2
13	-4	-7		8.7185	3.7827	1	3	-2	-3		5.3192	14.9078	2

$P2_1$	h	k	l	$F_{(obs)}$	$F_{(calc)}$	SF*
	3	-2	-2	37.5757	34.4113	2
	3	-2	0	13.7548	14.3315	2
	3	-3	-1	9.4129	10.0866	2
	4	-1	-1	50.7479	49.7643	2
	4	0	-2	119.9243	129.9369	2

\*Scale factor.