

Refinement of the crystal structure of celsian

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Abstract

The crystal structure of celsian from Jakobsberg, Sweden, ($\text{Ba}_{0.95}\text{K}_{0.05}\text{Al}_{1.95}\text{Si}_{2.05}\text{O}_8$, $a = 8.622$, $b = 13.078$, $c = 14.411$ Å, $\beta = 115.09^\circ$, space group $I2/c$) has been refined using 528 'a' reflections ($h+k$ even, l even) and 272 'b' reflections ($h+k$ odd, l odd) $> 1\sigma$. The 'b' reflections were measured at one-quarter the rate of 'a' reflections to obtain a higher level of significance for these very much weaker 'difference' reflections whose intensities are related only to Al/Si ordering in the tetrahedral framework.

The Jakobsberg celsian is very similar to a celsian from Broken Hill, Australia, ($\text{Ca}_{\sim 84}\text{Or}_{\sim 18}$) refined by Newnham and Megaw (1960). The mean T-O distances for the symmetrically non-equivalent tetrahedral sites are $T_1\text{O} = 1.639$, $T_2z = 1.636$; $T_1z = 1.719$, $T_2\text{O} = 1.718$ Å, indicating that by comparison with fully ordered anorthite the Si-rich sites contain ~ 0.18 Al and the Al-rich sites ~ 0.79 Al. In the Broken Hill celsian the Al contents are ~ 0.17 and ~ 0.76 , respectively, consistent with a somewhat lower Al/(Al+Si) ratio. These partially disordered Al/Si distributions are not in strict accord with the aluminum avoidance principle and may result from anti-phase domain textures as previously observed in bytownite and transitional anorthite.

Introduction

The first X-ray study of celsian ($\text{BaAl}_2\text{Si}_2\text{O}_8$, symbol: Cn) by Taylor *et al.*, (1934) showed it to be approximately isomorphous with the monoclinic K-feldspar orthoclase. Subsequently, Gay (1956) found that single crystal photographs of celsian showed a set of very weak diffraction maxima with $h+k$ odd, l odd, indicating that celsian is body-centered and that the c -dimension of its unit cell is ~ 14.4 Å, approximately twice that of the $C2/m$ orthoclase. The choice of the unconventional space group symbol $I2/c$ (cf. Fig. 1, Chiari *et al.*, 1975) was made by Newnham and Megaw (1960) in order to preserve the axial orientation of celsian relative to orthoclase and other feldspars, some of which also have been assigned unconventional space group symbols (albite and microcline, $C\bar{1}$; bytownite, $I\bar{1}$).

Newnham and Megaw (1960) solved the structure of a celsian (approximate formula $\text{Ba}_{0.84}\text{K}_{0.16}\text{Al}_{1.90}\text{Si}_{2.11}\text{O}_8$) from Broken Hill, Australia, using intensities from five zero-layer Weissenberg photographs taken about

the zones [100], [010], [001], [110], and [111]. They first determined the "average" structure, using only the strong 'a'-type reflections ($h+k$ even, l even) and refining in space group $C2/m$ with $c = 7.2$ Å. This symmetrized unit cell has the Ba atom and one oxygen (O_A2) on the mirror plane, one oxygen (O_A1) on the two-fold axis through the origin, and the two tetrahedrally coordinated Al, Si "average" atoms (T_1 and T_2) and the other oxygens O_B , O_C , O_D in general positions. Having refined the "average" or symmetrized structure, they continued the refinement in space group $I2/c$ by including the weak 'b' reflections ($h+k$ odd, l odd) and doubling the c cell edge. The Ba, O_A1 , and O_A2 atoms were shifted slightly from special to general positions. The tetrahedral and oxygen sites were "split" and given a notation which has since been simplified to $T_1\text{O}$, T_1z , $T_2\text{O}$, T_2z ; O_BO , O_Bz ; O_CO , O_Cz ; O_DO , O_Dz to indicate that they are related by a pseudo- $c/2$ translation in the doubled cell.²

Newnham and Megaw found that the mean T-O

² This notation is modified somewhat and simplified from that suggested by Megaw (1956). It corresponds to that used by Chiari *et al.* (1975).

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IQ IS SCALE NUMBER, IL IS POSITIVE FOR ACCEPTANCE OF DATUM, Q IS CALC F**2/SIN 2 THETA
 0 H K L Y(OBS) Y(CALC) A B OBS-CALC SIG(I) (O-C)/SIG(I) IQ IL Q EXTING

-9	1	4	48.7214	45.0298	-45.0298	3.6916	3.7718	0.9787	1	1	2191.30	1.0
-9	1	8	238.9219	236.5439	236.5439	2.3780	3.8494	0.6178	1	1	61131.59	1.0
-9	1	6	67.0032	62.1252	62.1252	4.8780	2.9806	1.6365	1	1	4254.98	1.0
-9	3	8	83.1139	75.4723	79.4723	3.6416	2.7275	1.3352	1	1	6707.54	1.0
-9	3	6	154.6654	153.3121	153.3121	1.3533	2.9752	0.4549	1	1	25181.17	1.0
-8	6	6	35.6743	33.4197	33.4197	2.2546	4.7997	0.4697	1	1	1226.00	1.0
-8	6	6	100.4008	98.1796	98.1796	2.2213	2.5582	0.8683	1	1	10789.97	1.0
-8	6	4	119.9091	112.9891	112.9891	6.5200	2.6174	2.6438	1	1	14149.46	1.0
-8	6	2	169.0137	169.1477	169.1477	-0.1340	3.0394	-0.0441	1	1	30514.96	1.0
-8	4	10	179.9438	178.0740	-178.0740	1.8698	3.0919	0.6048	1	1	35666.39	1.0
-8	4	8	20.3899	48.8631	-48.8631	-28.4732	11.5308	-2.4693	1	1	2827.01	1.0
-8	4	4	192.7637	194.1404	194.1404	-1.3767	3.2411	-0.4248	1	1	45592.86	1.0
-8	4	4	93.3033	93.9785	93.9785	2.2645	2.7854	0.8721	1	1	10568.14	1.0
-8	4	2	118.5336	116.2691	116.2691	4.1892	2.5968	0.2424	1	1	15511.30	1.0
-8	4	2	81.9600	77.7714	77.7714	0.3640	2.7771	1.5085	1	1	6479.03	1.0
-8	2	12	151.4743	151.8571	-151.8571	-2.5681	2.8579	-0.1339	1	1	25061.62	1.0
-8	2	10	216.4751	214.5102	-214.5102	1.9649	3.5282	0.5569	1	1	54188.51	1.0
-8	2	8	45.5624	43.4792	-43.4792	2.0832	3.6421	0.5720	1	1	2350.60	1.0
-8	2	6	206.4026	204.7323	204.7324	1.6703	3.4072	0.4902	1	1	53316.56	1.0
-8	2	4	240.1883	239.8243	239.8243	0.3640	3.8706	0.0941	1	1	72319.94	1.0
-8	2	2	77.3443	74.2133	74.2133	3.1310	2.6824	1.1672	1	1	6624.10	1.0
-8	2	0	53.9393	56.5074	-56.5074	0.6223	3.6578	0.1661	1	1	3571.86	1.0
-8	0	12	228.8854	228.2631	-228.2631	11.4003	3.7469	2.6259	1	1	57448.93	1.0
-8	0	10	36.3428	24.9425	-24.9425	-5.2176	4.3415	-1.5351	1	1	744.38	1.0
-8	0	8	82.1633	87.3809	87.3809	10.1361	3.3989	0.8782	1	1	9656.50	1.0
-8	0	6	13.7203	3.5843	3.5843	-6.7052	11.5423	-1.8780	1	1	16.63	1.0
-8	0	4	210.4969	209.3218	209.3218	-2.0879	3.4422	-0.6065	1	1	60349.65	1.0
-8	0	2	207.2340	209.3218	209.3218	-2.0676	3.6722	-0.5630	1	1	3245.52	1.0
-7	1	14	52.9977	55.0654	55.0654	1.3340	2.4264	0.5498	1	1	10270.36	1.0
-7	1	12	93.4992	92.1652	92.1652	-0.3448	4.1906	-0.0823	1	1	1833.20	1.0
-7	1	10	36.6039	36.9487	-36.9487	0.4581	3.6749	0.1247	1	1	76785.56	1.0
-7	1	8	229.4440	229.9022	-229.9022	0.0718	2.4855	0.0289	1	1	22905.07	1.0
-7	1	6	122.9668	122.8950	-122.8950	-0.4086	2.3945	-0.1707	1	1	11372.44	1.0
-7	1	4	86.1511	86.5597	-86.5597	3.7908	2.4302	1.5599	1	1	16173.73	1.0
-7	1	2	109.1807	105.3899	105.3899	0.1749	4.7913	0.0372	1	1	11372.44	1.0
-7	1	0	300.8535	300.6785	300.6787	1.1679	2.6470	0.3123	1	1	24833.66	1.0
-7	3	12	16.4239	14.9594	14.9594	0.8267	2.6470	0.3123	1	1	262.08	1.0
-7	3	10	139.2973	138.4706	-138.4706	1.1679	4.1279	-1.1843	1	1	54680.52	1.0
-7	3	8	199.0761	197.9082	-197.9082	-4.8888	4.1279	-1.1843	1	1	962.00	1.0
-7	3	6	261.2051	266.0938	-266.0940	4.8888	4.1279	-1.1843	1	1	962.00	1.0
-7	3	4	27.9480	32.9015	32.9015	-4.9535	5.6616	-0.8749	1	1	1375.35	1.0
-7	3	2	166.4448	166.7307	166.7307	-0.2859	2.9085	-0.0983	1	1	38895.91	1.0
-7	3	0	68.2515	65.8390	65.8390	2.4125	2.8358	0.8507	1	1	5633.26	1.0
-7	5	10	54.4595	51.3129	-51.3129	3.1467	3.1999	0.9833	1	1	3186.77	1.0
-7	5	8	97.3126	94.6542	-94.6542	2.6584	2.3919	1.1114	1	1	11615.18	1.0
-7	5	6	310.4282	309.4773	-309.4773	0.9509	4.8245	0.1971	1	1	128850.00	1.0
-7	5	4	74.9274	73.0619	-73.0620	1.8655	2.6049	0.7162	1	1	7186.48	1.0
-7	5	2	201.6973	198.8806	198.8806	2.8167	3.3453	0.8420	1	1	51382.21	1.0
-7	5	0	178.4869	176.7494	176.7494	1.7375	3.1048	0.5596	1	1	37928.52	1.0
-7	7	10	56.6694	58.1718	-58.1718	-1.5024	3.4302	-0.4380	1	1	3734.47	1.0
-7	7	8	180.8735	180.5367	-180.5367	0.3368	3.1110	0.1083	1	1	38242.37	1.0
-7	7	6	100.1828	99.7225	-99.7226	0.3368	3.1110	0.1083	1	1	38242.37	1.0
-7	7	4	100.1828	99.7225	-99.7226	0.3368	3.1110	0.1083	1	1	38242.37	1.0
-7	7	2	100.1828	99.7225	-99.7226	0.3368	3.1110	0.1083	1	1	38242.37	1.0
-7	7	0	100.1828	99.7225	-99.7226	0.3368	3.1110	0.1083	1	1	38242.37	1.0

EXTING

7	100.1828	99.7225	-99.7226	0.0	0.4603	2.4643	0.1868	1	1	1	1	12055.96	1.0
7	46.5935	47.5729	-47.5729	0.0	-0.9794	3.7996	-0.2578	1	1	1	1	2745.40	1.0
7	106.9943	105.3408	105.3408	0.0	1.6535	2.5393	0.6512	1	1	1	1	13043.32	1.0
7	216.0962	213.2008	213.2008	0.0	2.8954	3.6567	0.7918	1	1	1	1	50303.04	1.0
9	59.8767	61.5142	-61.5142	0.0	-1.6375	3.3900	-0.4831	1	1	1	1	4063.73	1.0
9	26.6120	8.2481	-8.2481	0.0	18.3639	6.3071	2.9116	1	1	1	1	73.10	1.0
6	86.9117	86.1747	86.1748	0.0	-0.7370	2.8781	0.2561	1	1	1	1	7916.22	1.0
10	86.1573	86.7328	-86.7328	0.0	-0.5754	2.6711	-0.2154	1	1	1	1	8342.32	1.0
10	226.8059	220.0318	-220.0318	0.0	6.7741	3.6997	1.8310	1	1	1	1	54287.32	1.0
10	130.6795	131.9816	-131.9816	0.0	-1.3021	2.7065	-0.4811	1	1	1	1	19174.52	1.0
6	33.0591	37.7575	37.7575	0.0	-4.6984	5.4645	-0.8598	1	1	1	1	1616.00	1.0
8	53.2680	51.4677	51.4677	0.0	1.8003	3.2509	0.5538	1	1	1	1	3236.32	1.0
8	100.6489	102.8384	102.8384	0.0	-2.1894	2.4846	-0.8812	1	1	1	1	13538.10	1.0
8	195.2009	197.0907	-195.0908	0.0	0.1101	3.2546	0.0338	1	1	1	1	49367.12	1.0
8	197.6348	197.4440	-197.4440	0.0	0.1909	3.2939	0.0579	1	1	1	1	49466.71	1.0
8	98.1329	92.1095	-92.1095	0.0	6.0234	2.6775	2.2496	1	1	1	1	10195.30	1.0
6	105.9568	111.8101	111.8101	0.0	-5.8532	3.0961	-1.8905	1	1	1	1	14218.98	1.0
6	285.4048	287.4377	287.4380	0.0	-2.0330	4.4804	-0.4537	1	1	1	1	104806.44	1.0
6	142.4862	145.6172	145.6172	0.0	-3.1310	2.7528	-1.1374	1	1	1	1	29329.78	1.0
6	139.5867	138.3758	-138.3758	0.0	1.2110	2.5900	0.4676	1	1	1	1	27976.43	1.0
6	253.9609	255.3746	-255.3746	0.0	-1.4137	4.0381	-0.3501	1	1	1	1	96782.88	1.0
6	172.7356	171.1059	-171.1059	0.0	1.6297	2.9560	0.5513	1	1	1	1	42334.07	1.0
6	40.2741	32.5249	32.5249	0.0	7.7493	4.3752	1.7712	1	1	1	1	1138.46	1.0
6	116.2769	120.0380	120.0380	0.0	-3.7611	2.5602	-1.4691	1	1	1	1	17738.11	1.0
4	214.1829	214.7299	214.7299	0.0	-0.5470	3.4848	-0.1570	1	1	1	1	64064.50	1.0
4	17.1553	16.0332	16.0332	0.0	1.1222	8.1653	0.1374	1	1	1	1	393.89	1.0
6	150.3685	150.7283	-150.7284	0.0	-3.3599	2.6454	-0.1360	1	1	1	1	37076.86	1.0
4	55.3755	54.2652	-54.2653	0.0	1.1103	2.8026	0.3962	1	1	1	1	4893.58	1.0
4	326.3638	324.1465	-324.1467	0.0	2.2171	5.0381	0.4401	1	1	1	1	169422.94	1.0
6	183.5703	186.5545	-186.5545	0.0	-2.9841	3.1150	-0.9580	1	1	1	1	52169.40	1.0
4	96.3631	94.4299	94.4299	0.0	1.9333	2.5646	0.7548	1	1	1	1	10023.57	1.0
2	207.4498	206.5882	206.5883	0.0	0.4615	3.4230	0.1348	1	1	1	1	55522.71	1.0
2	106.0748	104.7480	104.7481	0.0	1.3268	2.3527	0.5639	1	1	1	1	16189.59	1.0
6	15.0578	13.3780	13.3780	0.0	1.6799	8.3685	0.2007	1	1	1	1	314.95	1.0
2	140.6768	139.1405	-139.1405	0.0	1.5363	2.5576	0.6007	1	1	1	1	34763.82	1.0
2	306.7603	307.0046	-307.0049	0.0	-0.2446	4.7472	-0.0515	1	1	1	1	163663.31	1.0
2	173.6399	173.5430	-173.5430	0.0	0.6969	3.0134	0.0322	1	1	1	1	48261.05	1.0
6	66.3106	61.1674	-61.1674	0.0	5.1432	2.8559	1.8009	1	1	1	1	4269.43	1.0
0	178.4853	176.6931	176.6932	0.0	1.7921	3.1614	0.5669	1	1	1	1	41188.89	1.0
0	278.3633	280.3677	280.3679	0.0	-2.0044	4.3528	-0.4605	1	1	1	1	118461.88	1.0
0	241.3130	243.3672	243.3672	0.0	-2.0542	3.8109	-0.5390	1	1	1	1	99626.38	1.0
6	77.1367	80.8661	-80.8661	0.0	-3.7295	3.8413	-0.9709	1	1	1	1	11823.09	1.0
6	487.0171	492.6995	-492.6997	0.0	-5.6822	7.3883	-0.7691	1	1	1	1	448204.94	1.0
4	68.4075	71.5770	-71.5771	0.0	-3.1695	2.4485	-1.2945	1	1	1	1	9135.27	1.0
0	161.5661	152.4268	152.4268	0.0	9.1393	3.4047	2.6843	1	1	1	1	38122.06	1.0
0	128.1762	125.2424	-125.2424	0.0	2.9338	2.5802	1.1370	1	1	1	1	18601.68	1.0
1	214.0201	215.0691	-215.0692	0.0	-1.0490	3.4814	-0.3013	1	1	1	1	64790.87	1.0
1	112.4123	114.6927	114.6927	0.0	-2.2803	2.3322	-0.9778	1	1	1	1	21664.67	1.0
1	286.0437	286.6191	286.6194	0.0	-0.5754	4.4332	-0.1298	1	1	1	1	156650.38	1.0
1	136.9963	142.7605	142.7605	0.0	-3.0247	2.4209	-2.3810	1	1	1	1	43482.43	1.0
1	174.8954	177.9202	177.9202	0.0	5.7642	2.8696	-1.0541	1	1	1	1	71270.44	1.0
1	24.6999	13.7661	13.7661	0.0	10.9337	4.3619	2.5066	1	1	1	1	417.94	1.0
1	184.6166	185.9809	-185.9810	0.0	-1.3643	3.0525	-0.4470	1	1	1	1	69815.94	1.0
3	141.9541	139.6482	-139.6483	0.0	2.3059	2.7385	0.8420	1	1	1	1	22417.59	1.0
3	77.4901	79.8208	-79.8209	0.0	-2.3307	2.5866	-0.9011	1	1	1	1	8591.52	1.0

(4) EXTING

I	H	K	L	A	B	CALC	SIG	(C)	SIG	IQ	IL	Q
-4	4	14	50.0665	48.0403	48.0403	0.0	2.0262	3.6903	0.5491	1	1	2636.00
-4	4	12	120.5290	118.9904	-118.9904	0.0	1.5305	2.5185	0.6109	1	1	19196.26
-4	4	10	326.0127	331.4692	-331.4692	0.0	-5.4566	5.0357	-1.0836	1	1	176715.13
-4	4	8	121.4999	123.2650	-123.2650	0.0	-1.7652	3.0828	-0.5726	1	1	26729.82
-4	4	6	23.3175	11.8912	11.8912	0.0	11.4263	4.4778	2.5518	1	1	306.31
-4	4	2	372.9365	374.5488	374.5491	0.0	-1.6122	5.6904	-0.2833	1	1	332756.44
-4	4	0	77.0206	92.7435	92.7436	0.0	-15.7230	3.7852	-4.1538	1	1	18974.70
-4	4	14	75.8457	75.1639	75.1639	0.0	0.6818	2.6879	0.2537	1	1	6762.11
-4	2	12	77.9734	75.5557	-75.5557	0.0	2.4178	2.5141	0.9617	1	1	8203.49
-4	2	10	276.4868	280.6060	-280.6062	0.0	-4.1193	4.3104	-0.9557	1	1	136343.25
-4	2	8	300.4272	304.3494	-304.3496	0.0	-3.9223	4.6411	-0.8451	1	1	192527.63
-4	2	6	45.2577	41.2116	41.2116	0.0	4.0861	2.4408	1.6741	1	1	4143.83
-4	2	4	350.6902	351.1924	351.1929	0.0	-0.5024	5.3519	-0.0939	1	1	333637.38
-4	2	2	225.0633	230.6489	230.6489	0.0	-5.5855	3.5357	-1.5798	1	1	145154.63
-4	2	0	48.4211	45.2324	45.2325	0.0	3.1887	2.5334	1.2587	1	1	5103.14
-4	0	14	93.3432	87.7431	-87.7431	0.0	5.6001	2.4549	2.2812	1	1	9365.42
-4	0	12	165.3737	162.4414	-162.4414	0.0	2.9323	2.8460	1.0303	1	1	38700.86
-4	0	10	44.3001	45.7378	45.7378	0.0	-1.4376	3.2630	-0.4406	1	1	3719.25
-4	0	8	176.2384	182.4379	-182.4378	0.0	-6.1994	3.0447	-2.0361	1	1	71631.00
-4	0	6	225.3747	221.0146	-221.0146	0.0	4.3601	3.5391	1.2320	1	1	124704.31
-4	0	4	321.8828	319.1062	319.1064	0.0	2.7764	4.9269	0.5635	1	1	290798.50
-4	0	2	348.8057	345.1040	345.1042	0.0	3.7017	5.3239	0.6953	1	1	343344.25
-4	0	0	419.3058	419.0171	419.0173	0.0	0.2927	6.3806	0.0459	1	1	459021.38
-3	1	14	140.6490	135.4290	135.4291	0.0	5.2199	2.7271	1.9141	1	1	22193.93
-3	1	12	300.7683	298.6011	298.6013	0.0	2.1671	4.6821	0.4629	1	1	131830.94
-3	1	10	5.2118	1.2645	1.2645	0.0	3.9473	23.9271	0.1650	1	0	2.93
-3	1	8	103.9417	103.2013	-103.2013	0.0	0.7204	2.0665	0.3486	1	1	2454.16
-3	1	6	174.1170	183.3408	-183.3408	0.0	-9.2238	2.8183	-3.2729	1	1	97954.44
-3	1	4	311.0647	326.8557	-326.8562	0.0	-15.7910	4.7631	-3.3153	1	1	380639.75
-3	1	2	249.8125	35.8590	-35.8590	0.0	-3.2398	2.7708	-1.1593	1	1	4956.61
-3	1	0	212.9224	255.6028	255.6028	0.0	-5.7903	3.8890	-1.4889	1	1	227965.31
-3	3	12	102.6313	207.3624	207.3625	0.0	5.5600	3.5125	1.5829	1	1	50358.38
-3	3	10	68.1389	97.4332	97.4332	0.0	5.1981	2.8171	1.8452	1	1	13476.34
-3	3	8	167.1096	66.7209	66.7209	0.0	1.4180	2.4118	0.5880	1	1	7728.46
-3	3	6	288.0049	172.2103	-172.2104	0.0	-5.1007	2.7971	-1.8235	1	1	63399.33
-3	3	4	267.4238	289.5229	-289.5232	0.0	-1.5181	4.4406	-0.3419	1	1	219447.56
-3	3	2	189.2663	256.2166	-256.2168	0.0	11.2073	4.1213	2.7193	1	1	202021.44
-3	3	0	169.1905	186.7720	-186.7720	0.0	2.4942	3.0247	0.8246	1	1	113947.63
-3	3	14	112.5947	109.7204	109.7205	0.0	10.1607	3.5272	2.8807	1	1	76579.38
-3	3	12	74.2795	73.6298	73.6299	0.0	2.8743	2.6499	1.0847	1	1	13283.17
-3	3	10	191.5750	192.2715	192.2715	0.0	0.6497	2.6142	0.2485	1	1	7136.00
-3	3	8	99.1839	101.6712	-101.6712	0.0	-0.6965	3.1680	-0.2199	1	1	58237.91
-3	3	6	351.2136	352.1736	-352.1738	0.0	-2.4873	2.1532	-1.1551	1	1	19438.25
-3	3	4	243.1120	245.1286	-245.1286	0.0	-0.9599	5.3745	-0.1786	1	1	273888.44
-3	3	2	136.7722	133.7570	-133.7571	0.0	-2.0166	3.7986	-0.5309	1	1	149289.25
-3	3	0	222.4202	215.1646	215.1646	0.0	3.0152	2.3764	2.2688	1	1	46300.87
-3	3	12	243.2162	242.2928	242.2928	0.0	0.92334	3.5218	2.0602	1	1	113726.81
-3	3	10	91.7298	92.5862	-92.5862	0.0	0.92334	3.9068	0.2364	1	1	69812.94
-3	3	8	142.2276	143.6858	-143.6858	0.0	-0.8564	2.3009	-0.3722	1	1	13788.06
-3	3	6	200.2989	200.8489	-200.8489	0.0	-1.4581	2.5370	-0.5747	1	1	37617.49
-3	3	4	25.2347	19.4954	-19.4954	0.0	-0.5500	3.2264	-0.1705	1	1	80068.38
-3	3	2	156.0933	157.8938	-157.8938	0.0	5.7393	4.3747	1.3119	1	1	776.05
-3	3	0	61.6173	67.3492	-67.3492	0.0	-1.8005	2.6992	-0.6670	1	1	49088.93
-3	9	10	122.5767	124.4353	-124.4353	0.0	-5.7319	3.2151	-1.7828	1	1	5473.59
-3	9	8	Y(OBS)	Y(CALC)	A	B	CALC	SIG	(C)/SIG	IQ	IL	Q
												21072.49
												EXTING

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1 H K L

77.3002	79.7541	-79.7541	0.0	-2.4539	3.3553	-0.7313	1	9545.84
229.5791	224.1686	-224.1687	0.0	5.4104	3.6616	1.4776	1	80412.81
61.1106	64.2999	-64.3000	0.0	-3.1894	2.7089	-1.1774	1	6754.14
140.1855	137.2298	137.2298	0.0	2.9557	2.6617	0.1104	1	29958.43
56.0430	53.7843	-53.7844	0.0	2.2586	3.3204	0.6802	1	3324.64
247.6469	245.0211	-245.0211	0.0	2.6257	3.9449	0.6656	1	74624.13
257.4055	254.4197	-254.4197	0.0	2.9861	4.0700	0.7337	1	84580.13
71.0530	74.1851	-74.1852	0.0	-3.1322	2.7125	-1.1547	1	7305.83
210.3201	205.4852	205.4852	0.0	4.8349	3.4639	1.3958	1	54924.35
52.1845	49.9307	-49.9308	0.0	2.2538	3.4578	0.6518	1	2692.47
67.7417	63.8730	-63.8730	0.0	3.8687	2.8476	1.3586	1	4461.74
35.3984	32.6634	32.6634	0.0	2.7350	5.1200	0.5342	1	1148.08
103.3194	102.0380	102.0381	0.0	1.2814	2.5765	0.4973	1	11107.28
71.3148	67.8737	67.8737	0.0	3.4411	2.6991	1.2749	1	5336.69
71.5341	66.3967	-66.3967	0.0	5.1374	2.5860	1.9866	1	5408.91
251.3097	247.2503	-247.2503	0.0	4.0594	3.9910	1.0171	1	77034.19
59.9973	63.7369	-63.7369	0.0	-3.7397	3.2080	-1.1657	1	5082.70
172.6926	175.2012	175.2012	0.0	-2.5086	3.0510	-0.8222	1	34384.15
259.5002	265.5955	265.5957	0.0	-6.0954	4.1381	-1.4720	1	89207.19
10.5190	15.8628	-15.8628	0.0	-5.3439	14.2015	-0.3763	1	352.52
185.4861	186.3528	-186.3528	0.0	-0.8667	3.1576	-0.2745	1	52361.04
122.3575	117.9703	-117.9704	0.0	4.3871	2.3969	1.8304	1	21728.33
159.3942	155.2553	-155.2553	0.0	2.1390	2.8166	1.4695	1	37282.66
74.2623	77.1279	77.1279	0.0	4.1390	2.8166	-0.9615	1	6602.67
33.4221	17.9028	17.9028	0.0	15.5193	4.6996	3.3023	1	415.22
227.9810	233.6233	233.6233	0.0	-5.6423	3.6530	-1.5445	1	81937.94
161.4672	165.0596	165.0597	0.0	-3.5924	2.7775	-1.2934	1	46594.72
28.4069	16.3342	16.3342	0.0	12.0727	4.0630	2.9713	1	503.37
118.9528	117.5803	-117.5804	0.0	1.3725	2.2626	0.6066	1	27372.95
542.9600	527.3518	-527.3521	0.0	15.6082	8.2219	1.8984	1	543463.94
7.9818	14.7191	-14.7191	0.0	-6.7372	22.8894	-0.2943	1	268.30
249.4655	249.8382	249.8382	0.0	-0.3726	3.9539	-0.0942	1	92498.31
317.2710	326.9358	326.9360	0.0	-9.6647	4.9260	-1.9620	1	189584.00
95.3000	94.9240	94.9240	0.0	0.3760	2.0688	0.1817	1	18939.00
221.7961	217.9055	-217.9055	0.0	3.8906	3.5222	1.1046	1	114566.00
234.3542	232.1213	-232.1213	0.0	2.2329	3.6575	0.6105	1	139740.94
100.1369	99.7493	-99.7494	0.0	0.3876	2.3384	0.1657	1	25296.66
177.7395	171.6600	-171.6600	0.0	6.0795	3.0897	1.9677	1	32884.94
15.3631	24.2990	24.2990	0.0	-8.9359	10.6558	-0.8386	1	798.54
282.5103	285.1243	285.1245	0.0	-2.6141	4.4081	-0.5930	1	134871.81
99.0769	107.0578	107.0578	0.0	-7.9809	2.1720	-3.6745	1	23600.00
65.6172	73.5687	73.5687	0.0	-7.9515	2.0220	-3.9324	1	13912.52
74.4852	75.7192	-75.7192	0.0	-1.2340	1.8469	-0.6682	1	18034.84
454.8081	458.0947	-458.0950	0.0	-3.2867	6.8886	-0.4771	1	742832.69
122.7833	127.5079	-127.5079	0.0	-4.7245	2.2099	-2.1379	1	55646.64
43.3736	40.4285	-40.4286	0.0	2.9451	4.1622	0.7076	1	1908.97
60.5085	71.0473	71.0473	0.0	-10.5387	3.6763	-2.8667	1	7235.38
141.0299	140.5474	140.5474	0.0	0.4825	2.5351	0.1903	1	35403.96
178.0321	187.2164	187.2164	0.0	-9.1843	3.0485	-3.0128	1	80479.38
154.2324	157.0008	157.0008	0.0	-2.7684	2.5431	-1.0886	1	74590.63
322.9695	323.7461	-323.7463	0.0	-0.7767	4.9199	-0.1579	1	516303.13
531.6477	519.3391	-519.3394	0.0	12.3085	8.0266	1.5335	1	1250931.00
79.9584	77.9123	-77.9124	0.0	2.0461	2.7786	0.7364	1	7202.25
52.0804	51.1766	-51.1766	0.0	0.9037	3.3381	0.2707	1	3831.27
191.5012	196.5258	196.5258	0.0	-5.0246	3.1456	-1.5973	1	71171.06

OBS-CALC SIG(DD) (O-C)/SIG(DD) IQ II Q EXTING

	1	H	0	K	L	Y(OBS)	Y(CALC)	A	B	OBS-CALC	SIG(0)	(0-C)/SIG(0)	IO	IL	Q	EXTING
-2	0	0	8	603.6389	616.8945	616.8950	0.0	-13.2557	9.1123	-1.4547	1	1	910313.00	1.0		
-2	0	6	85.6813	79.4636	79.4637	0.0	6.2177	1.8665	1.8665	3.3312	1	1	20420.12	1.0		
-2	0	4	434.2061	435.7688	-435.7690	0.0	-1.5628	6.5726	6.5726	-0.2378	1	1	861109.63	1.0		
-2	0	2	33.0017	14.1209	14.1209	0.0	18.8808	2.1323	2.1323	8.8547	1	1	1175.30	1.0		
-1	0	0	306.6428	294.6699	-294.6702	0.0	11.9737	4.6786	4.6786	2.5593	1	1	471112.75	1.0		
-1	1	14	164.8566	159.5198	-159.5198	0.0	5.3369	3.0024	3.0024	1.7775	1	1	28768.68	1.0		
-1	1	12	241.2435	239.9447	-239.9448	0.0	1.2988	3.8810	3.8810	0.3347	1	1	80252.38	1.0		
-1	1	10	16.0202	21.9347	-21.9347	0.0	-5.9145	8.6458	8.6458	-0.6841	1	1	846.15	1.0		
-1	1	8	21.5907	8.0664	-8.0664	0.0	13.5242	4.9654	4.9654	2.7237	1	1	149.44	1.0		
-1	1	6	276.9263	281.0449	281.0452	0.0	-4.1187	4.2765	4.2765	-0.9631	1	1	250502.63	1.0		
-1	1	4	423.7095	433.2207	433.2209	0.0	-9.5111	6.4156	6.4156	-1.4825	1	1	902970.88	1.0		
-1	1	2	129.5526	121.2433	121.2433	0.0	8.3092	2.0747	2.0747	4.0050	1	1	120614.81	1.0		
-1	3	14	46.3398	43.6757	-43.6757	0.0	2.6641	4.1019	4.1019	0.6495	1	1	2093.96	1.0		
-1	3	12	111.5534	112.6720	-112.6721	0.0	-1.1186	2.5561	2.5561	-0.4376	1	1	17039.11	1.0		
-1	3	10	292.8198	297.0745	-297.0747	0.0	-4.2547	4.5620	4.5620	-0.9326	1	1	147477.56	1.0		
-1	3	8	53.0637	55.4470	-55.4471	0.0	-2.3833	2.5444	2.5444	-0.9367	1	1	6552.95	1.0		
-1	3	6	203.5424	215.6050	215.6051	0.0	-11.6627	3.2395	3.2395	-3.6002	1	1	130469.38	1.0		
-1	3	4	397.7266	409.2104	409.2109	0.0	-11.4838	6.0404	6.0404	-1.9012	1	1	638505.38	1.0		
-1	3	2	248.0585	237.8985	237.8985	0.0	10.1600	3.8172	3.8172	2.6616	1	1	285013.19	1.0		
-1	3	0	302.1240	272.5527	-272.5530	0.0	29.5713	4.6105	4.6105	6.4140	1	1	392694.81	1.0		
-1	5	12	129.8866	129.4439	-129.4440	0.0	0.4427	2.6361	2.6361	0.1679	1	1	20955.16	1.0		
-1	5	10	165.6555	169.5526	-169.5526	0.0	-3.8971	2.9044	2.9044	-1.3418	1	1	43795.56	1.0		
-1	5	8	61.3946	57.5955	57.5956	0.0	3.7990	2.4747	2.4747	1.5352	1	1	6222.69	1.0		
-1	5	6	151.5426	156.2841	156.2842	0.0	-4.7415	2.5819	2.5819	-1.8364	1	1	5681.68	1.0		
-1	5	4	233.3102	234.9506	234.9506	0.0	-1.6403	3.6491	3.6491	-0.4495	1	1	157634.13	1.0		
-1	5	2	257.7556	253.7439	253.7440	0.0	4.0117	3.9880	3.9880	1.0060	1	1	213188.38	1.0		
-1	5	0	87.8258	75.3599	-75.3599	0.0	12.4659	1.9535	1.9535	6.3813	1	1	19220.16	1.0		
-1	7	12	190.0174	191.2617	-191.2617	0.0	-1.2443	3.2483	3.2483	-0.3830	1	1	41570.36	1.0		
-1	7	10	73.0068	73.1612	-73.1613	0.0	-0.1545	2.7004	2.7004	-0.0572	1	1	7228.78	1.0		
-1	7	8	7.5443	14.7574	14.7574	0.0	-7.2131	19.1511	19.1511	-0.3766	1	0	349.61	1.0		
-1	7	6	252.4961	259.7981	259.7983	0.0	-7.3023	3.9721	3.9721	-1.8384	1	1	127793.38	1.0		
-1	7	4	298.8967	303.5977	303.5979	0.0	-4.7011	4.6104	4.6104	-1.0197	1	1	200925.00	1.0		
-1	7	2	105.4445	103.7718	103.7718	0.0	1.6727	2.0563	2.0563	0.8135	1	1	25687.13	1.0		
-1	7	0	8.7349	8.4955	-8.4955	0.0	0.2394	11.8389	11.8389	0.0202	1	0	174.32	1.0		
-1	9	10	73.7489	73.0989	-73.0990	0.0	0.6500	2.7835	2.7835	0.2335	1	1	6294.66	1.0		
-1	9	8	88.4244	89.4351	-89.4352	0.0	-1.0106	2.4609	2.4609	-0.4107	1	1	10868.30	1.0		
-1	9	6	176.7974	183.3180	183.3180	0.0	-6.5203	2.9981	2.9981	-2.1749	1	1	51923.09	1.0		
-1	9	4	379.3154	386.8677	386.8679	0.0	-7.5526	5.8022	5.8022	-1.3016	1	1	256144.75	1.0		
-1	9	2	54.0968	54.6086	54.6086	0.0	-0.5119	2.5740	2.5740	-0.1989	1	1	5425.93	1.0		
-1	9	0	155.0211	144.6446	-144.6447	0.0	10.3764	2.6382	2.6382	3.8630	1	1	38380.36	1.0		
-1	11	8	28.9502	22.1301	22.1301	0.0	6.8201	6.0586	6.0586	1.1257	1	1	562.14	1.0		
-1	11	6	63.7959	63.3477	63.3477	0.0	0.4482	2.8329	2.8329	0.1582	1	1	5103.20	1.0		
-1	11	4	148.3300	153.1579	153.1579	0.0	-4.8279	2.7057	2.7057	-1.7844	1	1	32252.47	1.0		
-1	11	2	154.1823	152.3626	152.3626	0.0	1.8197	2.7407	2.7407	0.6640	1	1	33389.43	1.0		
-1	11	0	31.7610	31.0041	-31.0041	0.0	0.7569	4.8793	4.8793	0.1551	1	1	1390.79	1.0		
-1	13	4	146.3609	146.6913	146.6913	0.0	-0.3304	2.7488	2.7488	-0.1202	1	1	24192.92	1.0		
-1	13	2	134.6758	134.6245	134.6245	0.0	0.0513	2.6501	2.6501	0.0194	1	1	21102.03	1.0		
-1	13	0	55.6741	55.0415	-55.0415	0.0	0.6326	3.5178	3.5178	0.1798	1	1	3543.51	1.0		
-1	14	0	123.3758	101.8482	101.8482	0.0	21.5276	4.5975	4.5975	4.6824	1	1	11093.59	1.0		
0	12	6	206.8205	217.3074	-217.3075	0.0	-10.4869	3.4855	3.4855	-3.0087	1	1	53496.23	1.0		
0	12	4	25.6983	23.5093	-23.5093	0.0	2.1890	7.3091	7.3091	0.2995	1	1	677.64	1.0		
0	12	2	185.3856	189.8570	189.8570	0.0	-4.4713	3.1786	3.1786	-1.4067	1	1	46522.27	1.0		
0	10	8	76.1729	97.4075	97.4075	0.0	-21.2346	7.5295	7.5295	-2.8202	1	1	12466.57	1.0		
0	10	6	161.1186	166.4291	-166.4291	0.0	-5.3105	2.9352	2.9352	-1.8092	1	1	33382.52	1.0		
0	10	4	131.7897	132.8820	-132.8821	0.0	-1.0924	2.5732	2.5732	-0.4245	1	1	24052.75	1.0		

0	10	4	112.5105	113.6977	-113.6977	0.0	-1.1871	2.3757	-0.4997	1	1	19473.74	1.0
0	10	2	115.1414	115.6914	115.6915	0.0	-0.5500	2.3569	-0.2334	1	1	21570.27	1.0
0	10	0	327.4182	331.3479	331.3481	0.0	-3.9297	5.2922	-0.7425	1	1	181225.19	1.0
0	8	10	120.0753	120.1649	-120.1649	0.0	-0.0896	2.6651	-0.0336	1	1	17392.10	1.0
0	8	8	349.3364	355.2151	-355.2156	0.0	-5.8788	5.4328	-1.0821	1	1	178527.50	1.0
0	8	6	1.2038	2.4106	-2.4106	0.0	-1.2068	120.3784	-0.0100	1	0	9.58	1.0
0	8	4	69.4857	69.6763	69.6764	0.0	-0.1905	2.8785	-0.0662	1	1	9147.95	1.0
0	8	2	75.1537	78.6012	78.6012	0.0	-3.4475	2.1212	-1.6253	1	1	12795.64	1.0
0	6	0	378.1692	373.6926	373.6929	0.0	4.4765	5.9290	0.7550	1	1	299458.00	1.0
0	6	12	36.0467	35.1442	-35.1442	0.0	0.9025	6.5341	0.1381	1	1	1396.84	1.0
0	6	10	57.2728	54.2941	-54.2941	0.0	2.9787	3.0935	0.9629	1	1	4010.45	1.0
0	6	8	72.9744	74.4901	-74.4902	0.0	-1.5158	2.5190	-0.6017	1	1	9144.21	1.0
0	6	6	236.0426	244.1269	-244.1269	0.0	-8.0842	3.7810	-2.1381	1	1	119313.13	1.0
0	6	4	191.6258	189.5214	-189.5215	0.0	2.1043	3.0943	0.6801	1	1	86507.94	1.0
0	6	2	251.2904	254.3771	254.3771	0.0	-3.0867	3.9150	-0.7884	1	1	180120.50	1.0
0	6	0	574.0496	541.3650	541.3652	0.0	32.6847	8.6688	3.7704	1	1	863905.69	1.0
0	4	10	214.1924	218.1847	-218.1848	0.0	-3.9924	3.5034	-1.1396	1	1	71578.31	1.0
0	4	8	165.7404	171.5323	-171.5323	0.0	-5.7919	2.8389	-2.0402	1	1	55361.81	1.0
0	4	6	331.5168	341.7246	-341.7249	0.0	-10.2079	5.0905	-2.0053	1	1	280999.81	1.0
0	4	2	322.1450	328.8320	328.8323	0.0	-6.6869	4.9296	-1.3565	1	1	435023.56	1.0
0	2	12	93.5707	94.6062	94.6062	0.0	-1.0355	2.6147	-0.3960	1	1	11522.18	1.0
0	2	10	202.1940	199.2651	-199.2651	0.0	2.9289	3.3196	0.8823	1	1	63840.74	1.0
0	2	8	352.8594	357.4585	-357.4587	0.0	-4.5991	5.4134	-0.8496	1	1	264083.63	1.0
0	2	6	159.2113	162.7687	-162.7687	0.0	-3.5575	2.6486	-1.3431	1	1	73614.38	1.0
0	2	4	105.6961	102.2375	102.2375	0.0	3.4586	1.9873	1.7403	1	1	41997.04	1.0
0	2	2	219.7115	213.4268	213.4268	0.0	6.2847	3.3925	1.8525	1	1	293434.31	1.0
0	2	0	269.3308	233.3524	233.3524	0.0	35.9786	4.0910	8.7946	1	1	498808.00	1.0
0	14	14	54.1692	13.0677	13.0677	0.0	41.1015	5.0545	8.1317	1	1	182.10	1.0
0	12	12	17.5798	9.7337	9.7337	0.0	7.8461	12.9259	0.6070	1	1	124.15	1.0
0	10	10	12.6416	9.1579	9.1579	0.0	3.4838	17.3398	0.2009	1	0	138.08	1.0
0	8	8	150.8278	157.1230	-157.1230	0.0	-6.2952	2.8390	-2.2174	1	1	52815.05	1.0
0	6	6	99.9459	107.7208	-107.7209	0.0	-7.7749	3.4090	-2.2807	1	1	34127.98	1.0
0	4	4	396.5281	393.4709	-393.4714	0.0	3.0571	6.0231	0.5076	1	1	698253.75	1.0
0	2	2	176.0488	161.2350	161.2350	0.0	14.8138	2.7305	5.4254	1	1	237638.38	1.0
1	12	12	157.9562	154.3489	154.3485	0.0	3.6073	2.9104	1.2394	1	1	28571.11	1.0
1	10	10	217.9806	219.6490	219.6490	0.0	-1.6684	3.5619	-0.4684	1	1	71761.06	1.0
1	8	8	157.9729	197.6232	197.6232	0.0	0.3497	3.2444	0.1078	1	1	73919.69	1.0
1	6	6	253.8753	249.8168	-249.8168	0.0	4.0584	3.9736	1.0214	1	1	156348.38	1.0
1	4	4	328.9670	343.9614	-343.9617	0.0	-14.9945	5.0397	-2.9753	1	1	418594.44	1.0
1	1	1	103.9851	103.9519	-103.9519	0.0	0.0332	1.9011	0.0174	1	1	60164.02	1.0
1	12	12	164.5674	158.8099	158.8099	0.0	5.7574	2.9561	1.9476	1	1	29306.64	1.0
1	10	10	132.4953	133.5739	133.5739	0.0	-1.0786	2.6172	-0.4121	1	1	25472.04	1.0
1	8	8	46.1524	44.7956	-44.7957	0.0	1.3568	3.2187	0.4215	1	1	3589.28	1.0
1	6	6	41.2634	40.8620	-40.8620	0.0	0.4014	2.9273	0.1371	1	1	3841.98	1.0
1	4	4	246.2608	240.2913	-240.2913	0.0	5.9695	3.8375	1.5556	1	1	176733.13	1.0
1	3	3	440.2666	444.4419	-444.4421	0.0	-4.1754	6.6756	-0.6255	1	1	824086.06	1.0
1	2	2	297.7375	272.5505	-272.5508	0.0	25.1869	4.5512	5.5341	1	1	392688.25	1.0
1	0	0	116.4259	113.1575	113.1575	0.0	3.2684	2.6929	1.2137	1	1	14015.32	1.0
1	5	10	289.1831	289.5481	289.5483	0.0	-0.3651	4.5462	-0.0803	1	1	110924.13	1.0
1	5	8	31.1052	30.2845	30.2846	0.0	0.8206	4.8342	0.1698	1	1	1482.91	1.0
1	5	6	155.2186	155.2679	-155.2679	0.0	-0.0493	2.6814	-0.0184	1	1	48130.06	1.0
1	5	4	272.2017	277.2788	-277.2791	0.0	-5.0772	4.2262	-1.2014	1	1	190301.31	1.0
1	5	2	319.3386	322.5388	-322.5391	0.0	-3.2002	4.8956	-0.6537	1	1	312941.19	1.0
1	5	0	91.4934	75.3557	-75.3557	0.0	16.1377	1.9153	8.4259	1	1	19218.01	1.0
1	7	10	177.7808	179.6804	179.6805	0.0	-1.8996	3.0985	-0.6131	1	1	38568.51	1.0

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EXITING

Table with columns labeled at the bottom: A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T, U, V, W, X, Y, Z. The table contains numerical data organized in rows. The bottom-most row contains the labels 'EXTING' and 'Q'. The right side of the page has some handwritten symbols and marks.

Y(OBS)	Y(CALC)	A	B	OBS-CALC	SIG(O)	(O-C)/SIG(O)	IO	IL	Q	EXTINC	
-8	12.3842	12.0087	-12.0087	0.0	0.3756	3.6808	0.1020	1	1	169.77	1.0
-8	12.0405	0.9434	-0.9434	0.0	11.0976	3.4766	3.1920	1	1	1.11	1.0
-8	8.3173	5.1138	5.1138	0.0	3.2035	5.0093	0.6395	1	1	33.65	1.0
-8	17.7063	8.0897	-8.0897	0.0	9.6165	2.9541	3.2553	1	1	83.73	1.0
-8	19.7783	14.1862	14.1862	0.0	5.5921	2.6527	2.1081	1	1	247.45	1.0
-7	10.7174	5.5192	5.5192	0.0	5.1982	3.7432	1.3887	1	1	42.22	1.0
-7	21.3429	24.6105	-24.6105	0.0	-3.2676	1.9591	-1.6679	1	1	890.85	1.0
-7	9.6951	0.3659	0.3659	0.0	9.3292	3.9044	2.3894	1	1	0.20	1.0
-7	18.0215	17.8125	17.8125	0.0	0.2086	2.1003	0.0993	1	1	465.96	1.0
-7	9.6645	1.6188	1.6188	0.0	8.0457	4.0687	1.9774	1	1	3.62	1.0
-7	15.6218	12.2911	-12.2911	0.0	3.3307	2.9496	1.1292	1	1	170.20	1.0
-7	10.6685	5.3329	5.3329	0.0	5.3356	3.7597	1.4191	1	1	39.50	1.0
-7	8.0148	6.5689	6.5689	0.0	1.0459	4.9528	0.2112	1	1	68.56	1.0
-7	15.7054	18.0339	-18.0339	0.0	-2.3285	2.7248	-0.8546	1	1	425.19	1.0
-7	18.8358	17.6279	17.6279	0.0	-1.2079	2.4992	0.4833	1	1	335.14	1.0
-7	11.7397	8.3166	8.3166	0.0	3.4231	3.7655	0.9091	1	1	83.28	1.0
-7	17.9419	17.9792	17.9792	0.0	-0.0373	2.3813	-0.0157	1	1	408.98	1.0
-7	18.0134	17.1223	-17.1224	0.0	0.8910	2.3463	0.3797	1	1	377.19	1.0
-7	9.4645	12.8199	-12.8199	0.0	-3.3555	4.4789	-0.7492	1	1	207.67	1.0
-7	5.7036	11.1635	11.1635	0.0	-5.4605	7.6290	-0.7157	1	0	149.69	1.0
-7	8.2341	1.7998	1.7998	0.0	6.4342	5.4623	1.1779	1	1	3.60	1.0
-7	7.8431	5.8104	-5.8104	0.0	2.0327	5.9181	0.3435	1	1	38.18	1.0
-7	11.9423	5.7232	-5.7232	0.0	6.2191	3.6061	1.7246	1	1	37.00	1.0
-7	12.9954	11.5820	11.5820	0.0	1.4135	3.6290	0.3895	1	1	144.93	1.0
-6	9.3328	6.4904	6.4904	0.0	2.8423	4.7927	0.5931	1	1	48.77	1.0
-6	10.9977	12.8993	-12.8993	0.0	-1.9017	8.9757	-0.2119	1	1	199.62	1.0
-6	14.9121	8.9479	8.9479	0.0	5.9642	2.8701	2.0780	1	1	96.45	1.0
-6	10.2899	7.2409	7.2410	0.0	3.0490	4.1771	0.7299	1	1	61.42	1.0
-6	15.5659	12.9780	-12.9780	0.0	2.5879	3.3983	0.7615	1	1	186.40	1.0
-6	2.2029	6.7464	-6.7464	0.0	-4.5435	19.1510	-0.2372	1	0	60.22	1.0
-6	3.6275	5.1964	-5.1964	0.0	-1.5689	11.3920	-0.1377	1	0	37.26	1.0
-6	13.3109	15.5573	-15.5573	0.0	-2.2464	3.0011	-0.7485	1	1	324.73	1.0
-6	16.3998	15.2362	15.2362	0.0	1.1636	2.6661	0.4364	1	1	291.39	1.0
-6	11.3339	15.6626	15.6626	0.0	-4.3286	3.9937	-1.0839	1	1	280.67	1.0
-6	7.9397	7.6381	-7.6381	0.0	0.3016	5.0716	0.0595	1	1	86.78	1.0
-6	7.1566	8.4635	8.4635	0.0	-1.3069	5.4097	-0.2416	1	1	111.92	1.0
-6	14.6857	11.8146	11.8146	0.0	2.8710	2.4504	1.1717	1	1	219.36	1.0
-6	7.2368	11.0728	-11.0728	0.0	-3.8360	5.6158	-0.6831	1	1	171.63	1.0
-6	8.2031	4.4714	-4.4714	0.0	3.7317	5.0814	0.7344	1	1	25.19	1.0
-6	17.2786	15.7895	15.7895	0.0	1.4891	2.6522	0.5615	1	1	277.74	1.0
-6	10.7191	6.6379	6.6379	0.0	4.0812	3.4452	1.1812	1	1	71.67	1.0
-6	15.4207	12.3287	-12.3287	0.0	3.0921	2.1659	1.4276	1	1	263.14	1.0
-6	7.8058	14.3441	14.3441	0.0	-6.5344	4.7085	-1.3878	1	1	340.86	1.0
-6	6.8857	2.1843	-2.1843	0.0	4.7013	5.7886	0.8122	1	1	7.25	1.0
-6	17.2862	10.2134	10.2134	0.0	7.0728	2.3662	2.9891	1	1	123.53	1.0
-6	8.3568	4.9596	-4.9596	0.0	3.3973	4.1462	0.8194	1	1	44.62	1.0
-6	24.0074	25.4512	-25.4512	0.0	-1.4439	1.4499	-0.9627	1	1	1183.45	1.0
-6	9.7276	8.9225	8.9225	0.0	0.8051	3.7393	0.2153	1	1	138.71	1.0
-6	26.7964	25.1462	26.1462	0.0	0.6503	1.4617	0.4449	1	1	1086.24	1.0
-6	8.4885	5.8204	5.8204	0.0	2.6680	4.5005	0.5928	1	1	47.63	1.0
-6	23.9451	24.3244	-24.3244	0.0	-0.3792	1.8837	-0.2013	1	1	723.68	1.0
-5	12.8940	14.0867	14.0867	0.0	-1.1927	2.3480	-0.5080	1	1	410.97	1.0
-5	9.9930	8.5787	8.5787	0.0	1.4143	2.9192	0.4845	1	1	160.96	1.0
-5	20.5904	22.7750	-22.7750	0.0	-2.1846	1.4708	-1.4853	1	1	1115.82	1.0
-5	8.7286	8.7753	-8.7753	0.0	-0.0467	3.4927	-0.0134	1	1	152.51	1.0

(11)

28.2615	27.7729	27.7729	0.0	0.4886	1.3642	0.3582	1	1	1	1343.90	1.0
9.3380	4.5480	4.5480	0.0	4.7900	3.9984	1.1980	1	1	1	30.95	1.0
21.1861	17.1652	-17.1653	0.0	4.0209	1.9333	2.0798	1	1	1	374.88	1.0
14.3629	12.1687	-12.1687	0.0	2.1941	2.3011	0.9535	1	1	1	279.12	1.0
6.3292	1.6154	1.6154	0.0	4.7138	4.8124	0.9795	1	1	1	5.16	1.0
18.2167	19.7746	19.7746	0.0	-1.5579	1.7693	-0.8805	1	1	1	761.67	1.0
8.0001	7.3688	-7.3688	0.0	0.6312	4.0353	0.1564	1	1	1	98.43	1.0
10.8868	9.8713	-9.8713	0.0	1.0155	3.3584	0.3024	1	1	1	157.60	1.0
5.6399	11.4968	-11.4968	0.0	-5.8572	6.2960	-0.9303	1	0	0	226.73	1.0
4.1768	8.1492	8.1492	0.0	-3.9724	8.3677	-0.4747	1	0	0	112.60	1.0
10.6957	10.6492	-10.6492	0.0	0.0465	3.6168	0.0129	1	1	1	164.41	1.0
10.2581	1.7916	1.7916	0.0	8.4666	3.9331	2.1527	1	1	1	4.12	1.0
6.6706	0.6067	0.6067	0.0	6.0640	6.7637	0.8965	1	1	0	0.41	1.0
7.7252	8.4614	8.4614	0.0	-0.7362	5.3029	-0.1388	1	1	1	101.42	1.0
17.9400	16.2641	-16.2642	0.0	1.6759	2.1512	0.7791	1	1	1	393.03	1.0
15.3912	17.2185	17.2185	0.0	-1.8273	2.6558	-0.6880	1	1	1	408.94	1.0
10.2713	4.5951	4.5951	0.0	5.6762	3.9364	1.4420	1	1	1	26.85	1.0
11.3277	12.6131	-12.6131	0.0	-1.2854	3.9271	-0.3273	1	1	1	182.15	1.0
15.3245	19.2169	19.2169	0.0	-3.8924	2.9373	-1.3252	1	1	1	457.03	1.0
14.2348	9.0479	-9.0479	0.0	5.1870	2.9378	1.7656	1	1	1	96.62	1.0
11.3554	5.3377	5.3377	0.0	6.0177	3.8457	1.5648	1	1	1	31.42	1.0
5.1922	6.2438	6.2438	0.0	-1.0515	8.4745	-0.1241	1	1	0	47.58	1.0
14.0174	12.6222	-12.6222	0.0	1.3952	3.0835	0.4525	1	1	1	197.15	1.0
10.3525	9.9945	9.9945	0.0	0.3580	4.1902	0.0854	1	1	1	121.25	1.0
7.8833	11.5330	-11.5330	0.0	-3.6498	5.0923	-0.7167	1	1	1	195.04	1.0
23.5919	26.0399	26.0399	0.0	-2.4479	1.7176	-1.4252	1	1	1	1011.88	1.0
16.6960	17.6210	-17.6210	0.0	-0.9250	2.3964	-0.3860	1	1	1	424.80	1.0
6.8448	9.8800	-9.8800	0.0	-3.0352	6.1612	-0.4926	1	1	0	121.74	1.0
2.9924	8.5299	-8.5299	0.0	-5.5374	11.6155	-0.4767	1	1	0	128.63	1.0
8.6501	8.5090	8.5090	0.0	0.1411	3.8954	0.0362	1	1	1	130.95	1.0
25.5246	25.6342	-25.6342	0.0	-0.1096	1.4683	-0.0746	1	1	1	1151.60	1.0
22.1905	23.2924	23.2924	0.0	-1.1019	1.8944	-0.5817	1	1	1	784.30	1.0
1.9747	10.8701	-10.8701	0.0	8.8954	21.7614	-0.4088	1	0	0	149.40	1.0
21.2578	18.5931	-18.5931	0.0	2.6647	2.2413	1.1889	1	1	1	378.29	1.0
5.0616	19.7557	-19.7557	0.0	1.4154	1.3920	1.0168	1	1	1	853.43	1.0
17.3738	8.0518	8.0518	0.0	-2.9902	5.6695	-0.5274	1	1	0	136.00	1.0
15.5929	16.3941	16.3941	0.0	0.9797	1.8131	0.5404	1	1	1	509.57	1.0
7.5453	18.3186	-18.3186	0.0	-2.7257	2.3998	-1.1358	1	1	1	553.99	1.0
3.6339	8.2025	-8.2025	0.0	-0.6573	5.2885	-0.1243	1	1	1	94.97	1.0
5.1884	9.8120	9.8120	0.0	-6.1781	12.5118	-0.4938	1	0	0	115.43	1.0
7.5381	7.1965	7.1965	0.0	-2.0081	5.2624	-0.3816	1	1	0	128.73	1.0
16.7538	1.6084	1.6084	0.0	5.9297	3.2883	1.8033	1	1	0	6.69	1.0
17.7791	17.4413	17.4413	0.0	-0.6875	1.6058	-0.4281	1	1	1	745.06	1.0
16.0942	15.3299	-15.3299	0.0	2.4492	1.5970	1.5336	1	1	1	507.44	1.0
5.9015	13.3194	-13.3194	0.0	2.7748	1.9733	1.4062	1	1	1	325.06	1.0
10.8939	10.0398	10.0398	0.0	-4.1384	6.5822	-0.6287	1	0	0	154.60	1.0
10.8469	6.1920	6.1920	0.0	4.7012	2.1442	2.1925	1	1	1	110.02	1.0
13.9761	10.6135	-10.6135	0.0	0.2333	2.3122	0.1109	1	1	1	303.38	1.0
25.62217	14.2400	-14.2400	0.0	-0.2640	1.8908	-0.1396	1	1	1	472.57	1.0
9.1668	25.6739	25.6740	0.0	-0.4522	1.3427	-0.3368	1	1	1	1280.70	1.0
21.6664	10.9531	10.9531	0.0	-1.7862	4.0832	-0.4375	1	1	1	192.51	1.0
5.2851	24.5760	-24.5760	0.0	2.3390	2.0471	-1.4213	1	1	1	802.38	1.0
5.1781	2.9461	2.9461	0.0	1.4713	4.3392	0.5390	1	1	1	30.45	1.0
5.0402	3.7068	-3.7068	0.0	0.7931	4.0885	0.3599	1	1	1	48.71	1.0
	4.2471	4.2471	0.0		4.4579	0.1779	1	1	1	55.72	1.0

1 H K L Y(OBS) Y(CALC) A B OBS-CALC SIG(O) (O-C)/SIG(O) IQ IL Q EXT INC

1	H	K	L	Y(OBS)	Y(CALC)	A	B	OBS-CALC	SIG(I)	(O-C)/SIG(I)	IQ	IL	Q	EXTING
-3	2	7	3.7355	8.2385	8.2385	0.0	-4.5030	6.8732	-0.6552	1	0	169.92	1.0	
-3	2	9	10.5027	9.6447	-9.6447	0.0	0.8579	2.8618	0.2998	1	1	186.23	1.0	
-3	2	11	3.5554	0.6440	-0.6440	0.0	2.9114	10.3670	0.2808	1	0	0.67	1.0	
-3	4	1	7.3737	4.7999	-4.7999	0.0	2.5738	3.2998	0.7800	1	1	65.97	1.0	
-3	4	5	8.4739	10.5754	10.5754	0.0	-2.1014	2.6938	-0.7801	1	1	322.60	1.0	
-3	4	3	7.6393	4.9041	-4.9041	0.0	-2.7353	3.1153	0.8780	1	1	62.79	1.0	
-3	4	9	2.9232	0.9752	0.9752	0.0	1.9481	11.0640	0.1761	1	0	1.74	1.0	
-3	4	13	15.2551	12.2518	12.2518	0.0	3.0032	2.8534	1.0525	1	1	187.64	1.0	
-3	6	1	8.1756	6.4228	-6.4228	0.0	1.7528	3.3205	0.5279	1	1	93.55	1.0	
-3	6	5	13.7938	14.6660	-14.6660	0.0	-0.8723	2.0616	-0.4231	1	1	457.20	1.0	
-3	6	7	8.5916	9.8064	-9.8064	0.0	-1.2149	3.6645	-0.3315	1	1	180.56	1.0	
-3	6	9	16.0597	16.8089	16.8089	0.0	-0.7492	2.5014	-0.2995	1	1	454.98	1.0	
-3	6	11	8.7147	9.9536	9.9536	0.0	-1.2388	4.7125	-0.2629	1	1	135.20	1.0	
-3	6	13	19.2890	15.9612	-15.9612	0.0	3.3277	2.3751	1.4011	1	1	293.83	1.0	
-3	8	1	2.8238	6.2225	-6.2225	0.0	-3.3987	12.1424	-0.2799	1	0	69.96	1.0	
-3	8	3	18.8121	19.2995	-19.2995	0.0	-0.4874	1.7323	-0.2814	1	1	675.38	1.0	
-3	8	5	11.0687	13.7200	13.7200	0.0	-2.6513	3.1409	-0.8441	1	1	324.60	1.0	
-3	8	7	4.2040	3.1808	3.1808	0.0	1.0232	8.5553	0.1196	1	0	15.88	1.0	
-3	8	9	9.2007	8.6202	-8.6202	0.0	0.5805	4.2487	0.1366	1	1	103.17	1.0	
-3	8	11	9.9682	8.5146	-8.5146	0.0	1.4535	4.3657	0.3329	1	1	87.55	1.0	
-3	10	3	3.2813	5.1897	5.1897	0.0	-1.9084	12.0316	-0.1586	1	1	39.44	1.0	
-3	10	5	10.2639	10.1804	-10.1804	0.0	0.0835	3.7621	0.0222	1	1	146.11	1.0	
-3	10	9	14.0777	14.8827	-14.8827	0.0	-0.8050	3.1238	-0.2577	1	1	262.87	1.0	
-3	12	5	20.4565	22.6234	-22.6234	0.0	-2.1669	2.2137	-0.9789	1	1	595.83	1.0	
-3	12	7	3.2824	4.0951	4.0951	0.0	-0.8127	14.2329	-0.0571	1	0	18.42	1.0	
-2	13	1	17.1103	16.5957	-16.5957	0.0	0.5146	2.6086	0.1973	1	1	314.10	1.0	
-2	13	3	15.3663	17.9268	17.9268	0.0	-2.5605	2.8925	-0.8852	1	1	363.29	1.0	
-2	13	5	12.5973	4.5947	-4.5947	0.0	8.0026	3.4878	2.2944	1	1	22.97	1.0	
-2	11	1	15.5040	13.5463	-13.5463	0.0	1.9578	2.5421	0.7701	1	1	256.96	1.0	
-2	11	3	13.3085	8.6222	8.6222	0.0	4.6863	2.8521	1.6431	1	1	172.93	1.0	
-2	11	7	9.2689	1.9230	-1.9230	0.0	7.3459	4.4526	1.6498	1	1	4.51	1.0	
-2	11	9	10.1552	13.5821	13.5821	0.0	-3.4269	4.6936	-0.7301	1	1	233.05	1.0	
-2	9	1	11.9792	14.5860	14.5860	0.0	-2.6067	2.8517	-0.9141	1	1	373.19	1.0	
-2	9	3	12.8453	10.6389	-10.6389	0.0	2.2064	2.5128	0.8780	1	1	195.53	1.0	
-2	9	5	13.1257	11.3670	11.3670	0.0	1.7588	2.7321	0.6437	1	1	209.37	1.0	
-2	9	7	16.9541	15.1074	15.1074	0.0	1.8468	2.2227	0.8309	1	1	334.15	1.0	
-2	9	9	26.9523	27.2245	-27.2245	0.0	-0.2722	1.7137	-0.1588	1	1	956.94	1.0	
-2	9	11	5.6619	3.1763	3.1763	0.0	2.4855	8.3645	0.2972	1	0	11.33	1.0	
-2	7	1	17.7716	18.5134	18.5134	0.0	-0.7418	1.5925	-0.4658	1	1	774.27	1.0	
-2	7	3	13.7299	16.4137	-16.4137	0.0	-2.6838	2.0357	-1.3183	1	1	595.25	1.0	
-2	7	5	11.2634	9.6384	-9.6384	0.0	1.6249	2.5553	0.6359	1	1	187.58	1.0	
-2	7	7	4.7336	7.2579	7.2579	0.0	-2.5242	7.2197	-0.3496	1	0	52.94	1.0	
-2	7	9	18.1480	15.7270	-15.7270	0.0	2.4211	2.1448	1.1288	1	1	372.86	1.0	
-2	7	13	22.9036	23.0892	-23.0892	0.0	-0.1855	2.2099	-0.0840	1	1	576.40	1.0	
-2	5	1	4.2226	8.0662	-8.0662	0.0	-3.8436	5.7208	-0.6719	1	0	196.61	1.0	
-2	5	3	4.5535	10.5822	10.5822	0.0	-6.0286	5.0884	-1.1848	1	0	326.60	1.0	
-2	5	5	10.1073	7.3217	-7.3217	0.0	2.7856	2.4060	1.1577	1	1	136.50	1.0	
-2	5	7	18.0077	16.3002	-16.3002	0.0	1.7075	4.4719	1.0806	1	1	562.31	1.0	
-2	5	9	7.8044	0.7253	0.7253	0.0	7.0791	4.4719	1.5830	1	1	0.91	1.0	
-2	3	1	14.1687	16.4668	-16.4668	0.0	-2.2981	1.5059	-1.5261	1	1	1140.54	1.0	
-2	3	3	14.8723	16.7793	16.7793	0.0	-1.9070	1.4117	-1.3509	1	1	1112.53	1.0	
-2	3	5	7.0333	3.7996	3.7996	0.0	3.2337	3.0630	1.0557	1	1	46.04	1.0	
-2	3	7	3.9381	0.3037	0.3037	0.0	3.6344	6.5125	0.5581	1	0	0.23	1.0	
-2	3	9	5.9645	4.7197	-4.7197	0.0	1.2448	5.3775	0.2315	1	1	43.29	1.0	
-2	3	11	5.4975	5.2066	-5.2066	0.0	0.2909	6.9874	0.0416	1	0	42.12	1.0	

3	4	7	7.6701	8.2821	8.2821	0.0	-0.6120	5.4952	-0.1114	1	1	101.02
3	4	9	9.5027	12.1634	-12.1634	0.0	-2.6607	5.0004	-0.5321	1	1	180.68
3	6	1	9.4882	3.0339	-3.0339	0.0	6.4543	3.1623	2.0410	1	1	19.31
3	6	5	8.0533	8.9104	8.9104	0.0	-0.8571	4.9527	-0.1731	1	1	125.25
3	6	7	8.4976	18.9983	-18.9983	0.0	-10.5007	5.2812	-1.9883	1	1	482.16
3	6	1	14.0010	13.1751	-13.1751	0.0	0.8259	2.6063	0.3169	1	1	296.42
3	6	7	7.7822	2.3488	-2.3488	0.0	5.4335	5.9439	0.9141	1	1	6.54
3	10	1	8.3637	7.4669	7.4669	0.0	0.8967	4.9160	0.1824	1	1	78.02
3	10	3	11.5054	6.3774	6.3774	0.0	5.1280	3.6980	1.3867	1	1	52.71
3	10	5	5.8416	7.9370	-7.9370	0.0	-2.0953	8.3184	-0.2519	1	1	73.71
3	12	1	9.5189	6.2374	6.2374	0.0	3.2815	4.7420	0.6920	1	1	45.03
3	12	1	11.3743	0.5384	0.5384	0.0	10.8359	4.6666	2.3220	1	1	0.32
4	9	1	7.1931	5.5881	-5.5881	0.0	-2.9563	6.3905	0.2512	1	1	36.41
4	9	3	6.5577	9.5140	-9.5140	0.0	-1.6284	6.7552	-0.4376	1	1	114.81
4	7	1	2.1114	3.3442	3.3442	0.0	-1.2328	17.5741	-0.0701	1	0	18.39
4	7	3	19.4378	21.0662	-21.0662	0.0	7.7481	2.2328	-0.7293	1	1	654.76
4	7	5	12.3572	4.6091	4.6091	0.0	3.8585	3.4006	2.2785	1	1	27.48
4	7	7	10.2494	6.3908	6.3908	0.0	1.0252	4.7409	0.8139	1	1	45.79
4	5	3	10.5752	9.5500	9.5500	0.0	5.0657	3.5697	0.2872	1	1	154.29
4	5	5	5.3293	0.2626	0.2626	0.0	-0.7045	7.7661	0.6523	1	0	0.10
4	3	3	9.4534	10.1579	10.1579	0.0	-5.8023	3.7379	-0.1885	1	1	194.52
4	3	5	5.6277	11.4300	-11.4300	0.0	-1.5451	7.1405	-0.8126	1	0	206.39
4	1	1	8.6637	10.2088	10.2088	0.0	-1.2931	3.2250	-0.4791	1	1	249.73
4	1	5	9.1828	10.4759	-10.4759	0.0	-0.2096	4.2568	-0.3038	1	1	181.74
4	1	7	11.9349	11.9445	11.9445	0.0	-3.9601	3.6012	-0.0027	1	1	195.45
4	1	9	4.6220	8.5820	8.5820	0.0	8.2114	10.6938	-0.3703	1	0	83.97
5	2	3	12.2942	4.0828	4.0828	0.0	-0.0236	3.1495	2.6072	1	1	26.78
5	2	5	13.6453	9.5083	9.5083	0.0	4.1370	3.1787	1.3015	1	1	123.92
5	4	1	9.5091	3.9928	-3.9928	0.0	5.5164	3.7441	1.4733	1	1	27.27
5	4	3	11.8531	7.0325	7.0325	0.0	4.8206	3.4090	1.4141	1	1	74.32
5	6	1	3.7515	3.7751	-3.7751	0.0	-1.8095	10.5419	-0.0022	1	0	21.68
5	6	3	6.0147	7.8243	7.8243	0.0	-2.2519	7.2907	-0.2482	1	0	83.24
5	6	5	10.5088	12.7607	-12.7607	0.0	10.1141	4.5797	-0.4917	1	1	194.24
5	8	5	10.9420	0.8279	-0.8279	0.0	0.1072	4.5253	2.2350	1	1	0.74
5	10	1	11.4013	11.2941	11.2941	0.0	-4.6396	4.1628	0.0257	1	1	145.54
6	9	1	7.8411	12.4807	-12.4807	0.0	-3.2571	6.1673	-0.7523	1	1	169.25
6	7	1	3.6240	6.8811	-6.8811	0.0	4.4563	12.5412	-0.2597	1	0	58.18
6	7	3	8.8250	4.3687	4.3687	0.0	1.4098	5.3361	0.8351	1	1	21.26
6	5	1	9.0225	7.6127	7.6127	0.0	4.4563	4.6431	0.3036	1	1	79.17
6	3	1	8.6312	2.7699	-2.7699	0.0	5.8613	5.4493	1.0756	1	1	10.05
6	3	3	8.0901	9.0904	9.0904	0.0	-1.0003	5.8428	-0.1712	1	1	94.45
6	3	5	4.5440	4.8139	-4.8139	0.0	-0.2699	8.8718	-0.0304	1	0	35.78
6	1	1	6.6430	5.3739	-5.3739	0.0	1.2692	6.6070	0.1921	1	1	39.24
6	1	3	19.0898	18.3311	-18.3311	0.0	0.7586	2.4077	0.3151	1	1	425.46
7	2	1	9.4545	13.1107	13.1107	0.0	-3.6562	5.1155	-0.7147	1	1	194.55
7	4	3	6.8173	7.2291	-7.2291	0.0	-0.4118	7.8274	-0.0526	1	0	56.61
7	6	1	17.6489	20.5454	20.5454	0.0	-2.8965	2.7372	-1.0582	1	1	470.64
8	1	1	12.3743	7.4304	-7.4304	0.0	4.9439	3.8724	1.2767	1	1	59.69

ICELSIAN REFINEMENT - 'A' AND 'B' REFLECTIONS ON SAME SCALE
 TIME FOR MATRIX SETUP WAS 0 SEC.
 NUMBER OF OBSERVATIONS ACCEPTED IS 800, NUMBER OF DEGREES OF FREEDOM IS 682
 NUMBER OF PARAMETERS VARIED IN THIS CYCLE WAS 118, TOTAL NUMBER OF PARAMETERS FITTED TO DATA SET TAKEN AS 118

***** MEASURES OF AGREEMENT BEFORE CYCLE 5 *****

***** MEASURES OF AGREEMENT BEFORE CYCLE 5 *****

	R(F)	R(F**2)	WR(YD)	SIG 1
FOR REFLECTIONS				
ACCEPTED BY LOGIC				
ALL INTENSITIES (800 REFLECTIONS)				
RATIO	0.0335	0.0391	0.0369	1.5963
NUMEPATOR	0.252869409E 04	0.755882688E 06	0.173790918E 04	
DENOMINATOR	0.873748750E 05	0.193089440E 08	0.127739500E 07	
GREATER THAN SIGMA (800 REFLECTIONS)				
RATIO	0.0335	0.0391	0.0369	1.5963
NUMERATOR	0.252869409E 04	0.755882688E 06	0.173790918E 04	
DENOMINATOR	0.873748750E 05	0.193089440E 08	0.127739500E 07	
NO TEST ON LOGIC				
ALL INTENSITIES (869 REFLECTIONS)				
RATIO	0.0371	0.0396	0.0447	1.8457
NUMERATOR	0.325369922E 04	0.764093438E 06	0.255829346E 04	
DENOMINATOR	0.877903750E 05	0.193154080E 08	0.127839700E 07	
GREATER THAN SIGMA (802 REFLECTIONS)				
RATIO	0.0345	0.0394	0.0446	1.9295
NUMERATOR	0.301941528E 04	0.760994188E 06	0.254647314E 04	
DENOMINATOR	0.874752500E 05	0.193140960E 08	0.127839500E 07	

ICELSIAN REFINEMENT - 'A' AND 'B' REFLECTIONS ON SAME SCALE
 ELEMENTS OF CORRELATION MATRIX OF MAGNITUDE GREATER THAN 0.30

SCALE	1	-	BA	B11	0.6321
		-	BA	B22	0.6283
		-	BA	B33	0.5996
		-	BA	B13	0.3573
BA	X	-	BA	Z	0.4100
BA	B11	-	BA	B33	0.3587
		-	BA	B13	0.5782
BA	B23	-	BA	B13	0.5984
BA	B12	-	BA	B23	0.5533
T10	X	-	T10	Z	0.5138
T10	B11	-	T10	B13	0.5392
		-	T1M	B11	-0.3644
T10	B22	-	T1M	B22	-0.3017
T10	B33	-	T10	B13	0.5413
		-	T1M	B33	-0.4170
T10	B12	-	T10	B23	0.5720
		-	T1M	B12	-0.4498
		-	T1M	B23	-0.3263
T10	B13	-	T1M	B13	-0.3417
T10	B23	-	T1M	B12	-0.3243
		-	T1M	B23	-0.4033
T1M	X	-	T1M	Z	0.5253
T1M	B11	-	T1M	B13	0.5268
T1M	B33	-	T1M	B13	0.4807
T1M	B12	-	T1M	B23	0.5706
T20	X	-	T20	Z	0.5490
		-	T2M	X	-0.3783
T20	Z	-	T2M	Z	-0.3049
T20	B11	-	T20	B13	0.5994
		-	T2M	B11	-0.3264
T20	B22	-	T2M	B22	-0.3431
T20	B33	-	T20	B13	0.5964
T20	B12	-	T20	B23	0.5774
		-	T2M	B12	-0.5104
		-	T2M	B23	-0.3254
T20	B13	-	T2M	B13	-0.3433
T20	B23	-	T2M	B12	-0.3314
		-	T2M	B23	-0.3984
T2M	X	-	T2M	Z	0.5526
T2M	B11	-	T2M	B13	0.5268

T1M	B11	-	T1M	B13	0.5268	
T1M	B33	-	T1M	B13	0.4807	
T1M	B12	-	T1M	B23	0.5706	
T20	X	-	T20	Z	0.5490	
		-	T2M	X	-.3783	
T20	Z	-	T2M	Z	-.3049	
T20	B11	-	T20	B13	0.5994	
		-	T2M	B11	-.3264	
T20	B22	-	T2M	B22	-.3431	
T20	B33	-	T20	B13	0.5964	
T20	B12	-	T20	B23	0.5774	
		-	T2M	B12	-.5104	
		-	T2M	B23	-.3254	
		-	T2M	B13	-.3433	
T20	B13	-	T2M	B12	-.3314	
T20	B23	-	T2M	B12	-.3984	
		-	T2M	B23	0.5526	
T2M	X	-	T2M	Z	0.5957	
T2M	B11	-	T2M	B13	0.5985	
T2M	B33	-	T2M	B13	0.5732	
T2M	B12	-	T2M	B23	0.5400	
OBO	X	-	OBO	Z	0.5582	
OBO	B11	-	OBO	B13	-.4043	
		-	OBO	B11	0.6056	
OBO	B33	-	OBO	B13	-.3108	
		-	OBO	B33	0.5437	
OBO	B12	-	OBO	B23	-.3833	
		-	OBO	B12	-.3472	
OBO	B13	-	OBO	B13	-.3163	
OBO	B23	-	OBO	B23	0.4687	
OBO	X	-	OBO	Z	0.5283	
OBO	B11	-	OBO	B13	0.5656	
OBO	B33	-	OBO	B13	0.4711	
OBO	B12	-	OBO	B23	0.5287	
OBO	X	-	OBO	Z	0.5383	
OBO	B11	-	OBO	B13	-.3548	
		-	OBO	B11	0.5045	
OBO	B33	-	OBO	B13	0.5675	
OBO	B12	-	OBO	B23	-.4212	
		-	OBO	B12	-.3194	
OBO	B13	-	OBO	B23	-.3342	
OBO	B23	-	OBO	B13	-.3193	
		-	OBO	B12	-.3118	
OBO	X	-	OBO	B23	0.5824	
OBO	B11	-	OBO	Z	0.5671	
OBO	B33	-	OBO	B13	0.5041	
OBO	B12	-	OBO	B13	0.5972	
OBO	X	-	OBO	B23	0.4913	
OBO	B11	-	OBO	Z	0.6051	
		-	OBO	B13	-.3240	
OBO	B33	-	OBO	B11	0.5827	
OBO	B12	-	OBO	B13	0.5450	
		-	OBO	B23	-.4030	
OBO	B13	-	OBO	B12	-.3422	
OBO	X	-	OBO	B12	0.5037	
OBO	B11	-	OBO	Z	0.6198	
OBO	B33	-	OBO	B13	0.6190	
OBO	B12	-	OBO	B13	0.5658	
OBO	X	-	OBO	B23	0.6282	
OBO	B11	-	OBO	Z	0.4657	
OBO	B33	-	OBO	B13	0.5293	
OBO	B12	-	OBO	B13	0.5710	
OBO	X	-	OBO	B23	0.4038	
OBO	B11	-	OBO	Z	0.4420	
OBO	B33	-	OBO	B13	0.5119	
OBO	B12	-	OBO	B13	0.5295	
OBO	X	-	OBO	B23		