

The following material did not appear in the original publication.

Table 2. Hydrochlorite. Brown and Clark

PAGE 20-1

H	M	X	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA F / SIGMA
-4	1	0	0	89.948	91.664	91.664	0.0	-1.716	0.558
-4	1	0	0	130.937	148.953	148.953	0.0	-18.016	3.007
-12	1	0	0	177.214	177.716	197.716	0.0	-20.502	1.786
-14	1	0	0	123.619	137.240	-137.240	0.0	-2.421	0.790
-14	1	0	0	237.847	239.510	-239.510	0.0	-17.440	5.671
-11	1	0	0	50.258	52.486	52.486	0.0	-2.202	0.716
-2	1	0	0	72.225	71.884	-51.884	0.0	0.284	0.208
-4	1	0	0	249.225	272.088	42.088	0.0	2.596	0.287
-4	1	0	0	113.447	24.732	-291.935	0.0	0.618	0.201
-4	1	0	0	123.964	110.704	43.173	0.0	-1.918	0.624
-4	1	0	0	181.773	120.510	120.510	0.0	2.739	0.891
-10	1	0	0	170.170	182.051	-182.051	0.0	3.476	1.130
-12	1	0	0	147.854	132.425	192.425	0.0	-11.812	0.329
-12	1	0	0	177.500	151.616	-151.616	0.0	-8.531	2.774
-14	1	0	0	237.817	237.737	237.737	0.0	-0.180	1.363
-14	1	0	0	232.307	225.560	225.560	0.0	6.747	3.529
-14	1	0	0	177.485	138.493	138.493	0.0	-3.992	1.045
-18	1	0	0	130.817	134.054	114.824	0.0	-1.233	0.355
-18	1	0	0	58.470	62.897	62.897	0.0	-4.427	1.428
-2	1	0	0	60.827	57.819	-57.819	0.0	3.008	0.578
2	1	0	0	9.656	8.731	-8.731	0.0	0.925	0.281
2	1	0	0	142.657	150.503	-150.503	0.0	-7.846	2.581
4	1	0	0	67.838	67.409	-67.409	0.0	0.429	0.139
4	1	0	0	78.109	76.757	-76.757	0.0	1.352	0.440
4	1	0	0	396.142	402.468	-402.468	0.0	-6.326	2.038
4	1	0	0	106.155	106.968	-106.968	0.0	-0.813	0.264
4	1	0	0	190.645	188.982	188.982	0.0	-1.663	1.617
4	1	0	0	54.307	58.261	-58.261	0.0	-3.954	0.349
4	1	0	0	98.128	90.577	-90.577	0.0	7.551	1.288
4	1	0	0	72.158	78.545	-78.545	0.0	-6.387	2.478
4	1	0	0	122.541	147.152	-147.152	0.0	-24.611	1.252
4	1	0	0	166.858	163.320	163.320	0.0	-3.538	0.225
4	1	0	0	37.908	32.046	-32.046	0.0	5.862	1.531
4	1	0	0	85.920	89.577	-89.577	0.0	-3.657	1.099
4	1	0	0	107.590	105.451	-105.451	0.0	2.139	1.889
4	1	0	0	65.693	68.566	-68.566	0.0	-2.873	0.588
4	1	0	0	65.101	52.768	-52.768	0.0	12.333	9.251
4	1	0	0	14.822	19.232	-19.232	0.0	4.410	1.033
4	1	0	0	155.522	153.304	153.304	0.0	-2.218	0.708
4	1	0	0	206.077	213.211	-213.211	0.0	-7.134	2.787
4	1	0	0	145.933	197.214	-97.214	0.0	-5.281	0.587
4	1	0	0	145.855	150.003	-150.003	0.0	-4.148	1.546
4	1	0	0	47.388	41.393	-41.393	0.0	5.995	1.649
4	1	0	0	207.081	210.050	-210.050	0.0	-2.969	0.565

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Table 2 (cont)  
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H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
-6	0	0	142.841	141.517	-141.517	0.0	1.324	0.431
8	0	0	142.131	140.274	-140.274	0.0	1.856	1.255
-8	0	0	229.707	229.152	-229.152	0.0	-6.448	-1.097
-10	0	0	195.597	195.115	-195.115	0.0	-3.482	-1.143
-12	0	0	190.509	191.694	191.694	0.0	1.185	0.232
-14	0	0	190.509	191.694	191.694	0.0	1.185	0.232
-14	0	0	130.377	114.743	-157.970	0.0	-157.970	-0.231
-15	0	0	183.491	177.262	-181.599	0.0	-5.229	-1.896
-15	0	0	119.285	36.865	-77.922	0.0	-1.544	-1.798
-18	0	0	54.769	118.183	119.121	0.0	17.355	5.719
-2	0	0	75.741	88.197	-56.197	0.0	-17.456	-1.565
0	0	0	58.574	56.418	-57.574	0.0	-1.156	-1.315
2	0	0	334.666	261.593	-52.073	0.0	-72.073	-0.242
4	0	0	355.910	355.910	0.0	0.0	0.0	0.0
4	0	0	112.822	113.720	113.720	0.0	0.898	0.340
5	0	0	160.705	160.949	-160.949	0.0	-0.244	-0.413
5	0	0	118.705	218.201	160.949	0.0	0.205	0.164
8	0	0	26.631	29.124	29.124	0.0	0.293	0.211
8	0	0	75.218	77.757	-77.757	0.0	-2.539	-0.281
8	0	0	99.759	75.317	-75.317	0.0	-24.442	-0.032
8	0	0	127.681	128.746	128.746	0.0	1.065	1.537
8	0	0	152.426	155.209	-155.209	0.0	-2.783	-0.227
8	0	0	102.350	100.999	-100.999	0.0	-1.351	-0.686
8	0	0	72.350	71.610	-71.610	0.0	-0.740	0.243
8	0	0	53.522	56.619	56.619	0.0	3.097	2.248
8	0	0	151.267	148.653	-148.653	0.0	-2.616	0.247
8	0	0	39.916	31.892	-31.892	0.0	-8.024	2.608
0	0	0	201.854	199.920	-199.920	0.0	-1.934	0.629
0	0	0	204.560	217.033	217.033	0.0	12.473	4.072
0	0	0	204.560	204.248	-204.248	0.0	-3.312	-0.121
0	0	0	106.768	110.599	110.599	0.0	3.831	1.298
0	0	0	47.420	46.124	-46.124	0.0	-1.296	-0.441
0	0	0	21.926	22.532	-22.532	0.0	-0.606	0.197
0	0	0	56.444	170.673	170.673	0.0	114.229	1.320
0	0	0	136.783	140.842	140.842	0.0	4.059	0.023
0	0	0	56.877	96.765	96.765	0.0	39.888	5.004
0	0	0	62.200	60.197	-60.197	0.0	-2.003	-0.655
0	0	0	7.822	23.231	23.231	0.0	15.409	0.828
0	0	0	54.823	225.990	225.990	0.0	171.167	1.971
0	0	0	47.200	97.555	97.555	0.0	50.355	0.654
0	0	0	45.677	39.057	-39.057	0.0	-6.620	-2.159
0	0	0	167.104	170.133	170.133	0.0	3.029	0.353
0	0	0	35.026	33.710	-33.710	0.0	-1.316	-0.734
0	0	0	137.060	145.622	145.622	0.0	8.562	0.958
0	0	0	225.544	225.476	-225.476	0.0	-0.068	-0.023
0	0	0	40.469	49.295	49.295	0.0	8.826	1.015
0	0	0	11.123	11.006	-11.006	0.0	-0.117	-0.037

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
5	0	12	175.985	175.100	175.100	0.000	-14.116	-4.590
5	0	12	174.780	174.975	-34.875	0.000	-10.095	-0.031
5	0	12	172.712	175.129	115.129	0.000	10.198	3.316
5	0	12	172.732	166.187	-66.187	0.000	-3.875	-0.778
5	0	12	174.648	176.002	99.681	0.000	2.049	1.260
5	0	12	24.402	26.722	26.722	0.000	-1.340	-0.436
5	0	12	27.870	30.404	30.404	0.000	-2.575	-0.870
5	0	14	27.870	61.404	61.404	0.000	3.092	0.976
5	0	14	30.812	25.072	-25.072	0.000	-8.736	-2.841
5	0	14	30.812	88.570	88.570	0.000	15.808	2.846
5	0	14	30.812	88.570	88.570	0.000	-12.183	-3.962
5	0	14	30.812	31.388	31.388	0.000	-12.051	-3.670
5	0	14	24.232	28.282	28.282	0.000	-7.154	-1.842
5	0	14	30.812	139.155	139.155	0.000	3.326	2.326
5	0	14	145.765	149.484	149.484	0.000	3.352	0.733
5	0	14	22.941	19.466	-19.466	0.000	-3.421	-1.155
5	0	15	19.466	19.466	19.466	0.000	3.475	1.210
5	0	15	38.101	39.230	39.230	0.000	10.426	3.390
5	0	15	155.634	158.324	158.324	0.000	1.139	0.370
5	0	15	127.772	133.301	133.301	0.000	-2.591	-0.875
5	0	15	17.867	23.774	23.774	0.000	-2.428	-1.798
5	0	15	229.745	276.566	276.566	0.000	-2.145	-0.698
5	0	15	147.545	153.013	153.013	0.000	-1.787	-0.451
5	0	15	45.742	54.716	54.716	0.000	-9.107	-1.506
5	0	15	37.056	34.555	-34.555	0.000	-2.373	-0.823
5	0	15	106.339	107.354	107.354	0.000	1.021	0.333
5	0	15	53.723	52.303	-52.303	0.000	-1.425	-0.462
5	0	15	50.925	50.920	-50.920	0.000	-0.042	-0.015
5	0	15	16.206	14.814	-14.814	0.000	1.082	0.453
5	0	15	2.6200	2.5773	-2.5773	0.000	-1.161	-0.353
5	0	15	17.950	2.668	-2.668	0.000	15.302	2.004
5	0	15	17.021	31.321	31.321	0.000	19.302	4.576
5	0	15	134.139	140.735	140.735	0.000	-6.598	-1.792
5	0	15	246.823	49.016	-49.016	0.000	-10.588	-2.822
5	0	15	78.823	240.659	240.659	0.000	6.175	1.702
5	0	15	92.653	82.596	-82.596	0.000	-3.072	-0.866
5	0	15	101.122	97.726	-97.726	0.000	-0.426	-0.120
5	0	15	102.424	101.771	-101.771	0.000	0.655	0.183
5	0	15	12.222	99.778	99.778	0.000	2.655	0.823
5	0	15	12.711	52.388	52.388	0.000	-10.116	-3.023
5	0	15	58.699	20.289	-20.289	0.000	-7.557	-2.458
5	0	15	71.429	39.598	-39.598	0.000	3.024	0.933
5	0	15	71.774	66.819	66.819	0.000	0.411	0.145
5	0	15	41.420	24.582	-24.582	0.000	6.477	2.145
5	0	15	41.420	72.584	72.584	0.000	-0.809	-0.283
5	0	15	41.269	85.537	85.537	0.000	-4.107	-1.374
5	0	15	41.269	-43.657	-43.657	0.000	-2.428	-0.750

Table 2 (cont.)  
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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	1	0	24.757	24.652	254.652	0.0	-9.285	-3.019
1	5	0	35.528	35.528	55.528	0.0	-0.174	-0.707
1	5	0	30.618	30.618	50.618	0.0	-0.850	-0.277
1	5	0	38.071	38.071	58.071	0.0	-7.521	-1.524
1	7	0	45.974	45.974	46.064	0.0	-0.090	-0.039
1	7	0	45.974	45.974	21.120	0.0	5.511	1.922
1	7	0	15.120	15.120	-134.402	0.0	2.738	0.890
1	7	0	34.572	34.572	34.570	0.0	0.014	0.655
1	7	0	33.549	33.549	-101.844	0.0	0.979	0.318
1	7	0	12.252	12.252	-122.969	0.0	-2.067	-0.672
1	7	0	72.252	72.252	-72.250	0.0	0.195	0.063
1	7	0	44.770	44.770	-44.771	0.0	0.811	0.811
1	7	0	37.444	37.444	-37.443	0.0	-4.762	-1.549
1	7	0	95.663	95.663	-95.663	0.0	1.057	0.244
1	7	0	31.793	31.793	31.793	0.0	-0.594	-0.226
1	7	0	48.622	48.622	48.622	0.0	-2.031	-0.660
1	7	0	53.278	53.278	53.278	0.0	-2.194	-1.039
1	7	0	27.278	27.278	-27.278	0.0	1.224	0.398
1	7	0	86.570	86.570	86.570	0.0	-0.803	-0.261
1	7	0	187.038	187.038	187.038	0.0	-2.959	-0.962
1	7	0	46.273	46.273	46.273	0.0	0.100	0.033
1	7	0	54.720	54.720	-54.720	0.0	-7.218	-2.347
1	7	0	171.742	171.742	-171.742	0.0	3.491	1.112
1	7	0	8.409	8.409	-8.409	0.0	1.916	0.546
1	7	0	172.319	172.319	172.319	0.0	-2.309	-0.784
1	7	0	79.540	79.540	79.540	0.0	5.744	1.825
1	7	0	4.002	4.002	-4.002	0.0	12.788	4.159
1	7	0	102.885	102.885	102.885	0.0	0.323	0.993
1	7	0	79.884	79.884	-79.884	0.0	-3.757	-1.222
1	7	0	91.553	91.553	91.553	0.0	-2.757	-0.856
1	7	0	22.000	22.000	22.000	0.0	-2.451	-0.774
1	7	0	159.513	159.513	-159.513	0.0	0.212	0.674
1	7	0	45.406	45.406	45.406	0.0	0.322	0.979
1	7	0	120.288	120.288	120.288	0.0	-1.074	-0.359
1	7	0	101.548	101.548	101.548	0.0	0.957	0.323
1	7	0	50.958	50.958	-50.958	0.0	-3.757	-1.092
1	7	0	190.911	190.911	-190.911	0.0	0.074	0.261
1	7	0	61.776	61.776	-61.776	0.0	-0.074	-0.261
1	7	0	19.157	19.157	19.157	0.0	0.074	0.261
1	7	0	123.696	123.696	123.696	0.0	-0.074	-0.261
1	7	0	182.225	182.225	182.225	0.0	0.074	0.261
1	7	0	219.203	219.203	-219.203	0.0	-0.074	-0.261
1	7	0	206.049	206.049	-206.049	0.0	0.074	0.261
1	7	0	212.559	212.559	212.559	0.0	-0.074	-0.261
1	7	0	116.004	116.004	-116.004	0.0	0.074	0.261
1	7	0	93.696	93.696	93.696	0.0	-0.074	-0.261
1	7	0	21.784	21.784	-21.784	0.0	0.074	0.261
1	7	0	77.653	77.653	-77.653	0.0	-0.074	-0.261
1	7	0	24.856	24.856	24.856	0.0	0.074	0.261
1	7	0	69.459	69.459	69.459	0.0	-0.074	-0.261

HCLB H REFINEMENT -ALL OTHERS FIXED ANISOTROPIC- CYCLE 32(9-22-77)										STRUCTURE FACTORS	
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA			
15	1	4	128.203	128.805	29.805	0.0	-1.601	-0.521			
17	1	4	88.918	158.712	58.712	0.0	4.206	1.358			
19	1	4	93.235	106.426	106.426	0.0	-7.191	-2.338			
21	1	4	93.202	85.454	85.454	0.0	13.556	4.402			
23	1	4	18.526	9.223	9.223	0.0	5.353	1.741	*		
25	1	4	123.417	99.991	-69.991	0.0	0.070	0.010	**		
27	1	4	123.417	190.782	190.782	0.0	0.237	0.077			
29	1	4	243.954	30.569	30.569	0.0	-5.153	-1.356			
31	1	4	212.894	25.881	-69.881	0.0	4.169	0.961			
33	1	4	212.894	23.973	245.673	0.0	0.321	0.097			
35	1	4	212.894	23.973	239.707	0.0	6.751	2.065			
37	1	4	135.030	142.698	51.189	0.0	2.883	0.938			
39	1	4	31.244	142.698	142.698	0.0	6.232	2.026			
41	1	4	55.539	75.055	40.848	0.0	-5.822	-1.893			
43	1	4	114.083	122.025	35.035	0.0	-3.811	-1.239			
45	1	4	114.083	148.047	148.047	0.0	-0.585	-0.190			
47	1	4	185.982	180.052	180.052	0.0	-2.164	-0.704			
49	1	4	142.076	180.052	180.052	0.0	5.529	1.928			
51	1	4	51.811	51.811	51.811	0.0	1.074	0.349			
53	1	4	40.451	40.451	40.451	0.0	0.159	0.052			
55	1	4	55.545	52.250	-24.750	0.0	4.277	1.391			
57	1	4	55.545	56.328	56.328	0.0	-2.069	-0.673			
59	1	4	50.296	19.142	19.142	0.0	3.014	1.143			
61	1	4	100.066	101.066	101.066	0.0	-1.154	-0.375			
63	1	4	92.870	89.634	-89.634	0.0	4.236	1.377			
65	1	4	74.419	75.645	75.645	0.0	-1.226	-0.399			
67	1	4	308.008	299.355	-299.355	0.0	1.422	0.483			
69	1	4	159.170	160.427	160.427	0.0	-1.256	-0.409			
71	1	4	61.811	58.899	58.899	0.0	2.312	0.947			
73	1	4	16.843	24.623	-24.623	0.0	-1.671	-0.555			
75	1	4	16.843	17.510	-17.510	0.0	3.084	1.024	**		
77	1	4	135.909	101.924	101.924	0.0	1.184	0.396			
79	1	4	31.151	29.966	29.966	0.0	1.627	0.544			
81	1	4	29.727	24.774	-24.774	0.0	7.840	2.523			
83	1	4	33.921	30.120	30.120	0.0	-1.223	-0.424			
85	1	4	85.459	87.070	87.070	0.0	-2.643	-0.866	**		
87	1	4	87.764	6.102	6.102	0.0	3.643	1.168			
89	1	4	57.930	54.530	54.530	0.0	24.782	8.023	**		
91	1	4	28.070	3.293	3.293	0.0	0.273	0.086			
93	1	4	11.440	10.335	10.335	0.0	0.115	0.033	**		
95	1	4	17.129	16.470	-16.470	0.0	2.650	0.824			
97	1	4	100.865	97.900	97.900	0.0	-0.544	-0.164			
99	1	4	39.547	41.453	41.453	0.0	-0.406	-0.132			
101	1	4	50.181	60.323	60.323	0.0	-0.142	-0.049			
103	1	4	255.915	256.772	256.772	0.0	7.851	2.564			
105	1	4	202.716	194.445	194.445	0.0	-0.124	-0.044			
107	1	4	97.021	97.145	-97.145	0.0	4.299	1.365	**		
109	1	4	17.682	4.617	-4.617	0.0					

Table 2 (cont)  
PAGE 40-5

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
1	1	7	49.449	51.915	51.915	0.0	-2.466	-0.802
1	1	7	72.020	66.765	-66.765	0.0	5.255	1.709
1	1	7	44.122	40.846	40.846	0.0	3.276	1.132
1	1	7	53.016	40.699	60.699	0.0	-7.683	-2.499
1	1	7	130.242	126.900	-126.900	0.0	10.342	3.351
1	1	7	137.477	95.746	-60.746	0.0	10.504	-0.164
1	1	7	137.913	30.484	95.484	0.0	11.993	3.900
1	1	7	57.530	57.530	30.022	0.0	0.010	4.273
1	1	7	25.1173	27.445	57.528	0.0	-2.328	0.003
1	1	7	194.504	18.435	247.445	0.0	3.734	1.214
1	1	7	162.740	180.628	18.438	0.0	-9.705	-3.156
1	1	7	164.214	161.222	189.628	0.0	4.876	1.586
1	1	7	28.722	27.522	151.622	0.0	-8.903	-2.895
1	1	7	59.156	56.728	161.222	0.0	2.428	0.961
1	1	7	166.800	162.128	-56.728	0.0	1.170	0.916
1	1	7	62.856	158.227	-158.227	0.0	-1.358	-0.441
1	1	7	21.210	6.575	98.257	0.0	4.630	1.505
1	1	7	121.060	56.926	-65.254	0.0	14.644	4.762
1	1	7	130.338	121.378	-121.378	0.0	0.493	-0.160
1	1	7	13.838	18.003	-18.003	0.0	-7.085	-0.087
1	1	7	19.167	49.897	-49.897	0.0	5.935	2.304
1	1	7	99.918	93.009	-93.009	0.0	6.909	2.036
1	1	7	7.842	19.974	-19.974	0.0	-3.131	-1.018
1	1	7	178.974	181.430	-181.430	0.0	-12.062	-3.922
1	1	7	26.692	15.226	-15.226	0.0	11.468	0.798
1	1	7	32.043	23.226	23.226	0.0	-8.817	-2.723
1	1	7	43.145	50.226	-50.226	0.0	7.081	2.845
1	1	7	130.356	126.334	126.334	0.0	-4.023	-2.309
1	1	7	32.166	36.722	-36.722	0.0	4.556	1.308
1	1	7	107.253	98.725	-98.725	0.0	-8.529	-1.475
1	1	7	34.965	67.053	-67.053	0.0	0.566	-0.064
1	1	7	66.823	29.052	29.052	0.0	-3.720	-1.916
1	1	7	41.361	32.027	75.952	0.0	-3.334	-2.568
1	1	7	32.280	30.274	30.274	0.0	2.015	0.655
1	1	7	80.169	74.781	74.781	0.0	-5.388	-1.752
1	1	7	25.616	23.175	-23.175	0.0	2.265	0.816
1	1	7	63.933	61.423	61.423	0.0	-2.510	-0.816
1	1	7	43.328	44.580	-44.580	0.0	-4.121	-0.407
1	1	7	95.028	80.907	80.907	0.0	-4.121	-0.407
1	1	7	72.697	74.154	-74.154	0.0	1.457	0.474
1	1	7	78.632	80.523	-80.523	0.0	-1.891	-0.645
1	1	7	24.600	23.433	-23.433	0.0	1.1778	0.420
1	1	7	23.310	27.227	-27.227	0.0	3.917	1.299
1	1	7	55.870	11.532	-11.532	0.0	5.664	1.850
1	1	7	173.888	59.006	-59.006	0.0	-1.379	-0.459
1	1	7	114.888	113.209	-113.209	0.0	1.679	0.566
1	1	7	83.767	79.170	79.170	0.0	-4.598	-1.420
1	1	7	24.786	24.242	24.242	0.0	0.544	0.177



Table 2 (cont)  
PAGE 207

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
13	1	10	52.135	54.768	54.768	0.0	4.368	1.420	
15	1	10	7.533	38.900	38.900	0.0	-1.467	-0.477	
17	1	10	14.117	4.373	4.373	0.0	9.742	3.168	**
4	1	11	3.335	142.535	142.535	0.0	2.582	0.840	
6	1	11	4.179	28.179	28.179	0.0	-6.715	-2.184	
8	1	11	3.335	41.065	41.065	0.0	-7.730	-2.514	
10	1	11	7.258	64.943	64.943	0.0	-6.136	-1.995	
12	1	11	62.089	84.402	84.402	0.0	-4.818	-1.567	
14	1	11	15.718	17.802	17.802	0.0	0.293	0.092	
16	1	11	40.008	38.036	38.036	0.0	-0.304	-0.099	
18	1	11	13.084	40.252	40.252	0.0	1.970	0.641	
20	1	11	152.190	143.752	143.752	0.0	0.239	0.270	
22	1	11	22.941	133.728	133.728	0.0	8.432	2.742	
24	1	11	25.278	22.027	22.027	0.0	-0.134	-0.044	
26	1	12	51.017	55.688	55.688	0.0	3.011	0.979	
28	1	12	23.402	22.830	22.830	0.0	-4.811	-1.584	
30	1	12	27.215	19.919	19.919	0.0	0.572	0.186	
32	1	12	40.162	36.885	36.885	0.0	7.297	2.373	
34	1	12	72.851	69.552	69.552	0.0	3.276	1.065	
36	1	12	19.466	5.895	5.895	0.0	3.299	1.073	
38	1	12	77.064	83.338	83.338	0.0	13.570	4.413	**
40	1	12	22.971	75.671	75.671	0.0	-16.217	-5.041	**
42	1	12	11.128	33.235	33.235	0.0	-4.342	-1.477	**
44	1	12	17.224	22.564	22.564	0.0	-22.011	-7.158	**
46	1	12	66.085	61.883	61.883	0.0	-15.184	-4.938	**
48	1	12	30.505	33.480	33.480	0.0	4.302	1.367	**
50	1	13	11.132	16.446	16.446	0.0	-2.574	-0.967	**
52	1	13	53.692	68.217	68.217	0.0	5.314	1.728	**
54	1	13	59.468	66.020	66.020	0.0	-14.324	-4.723	**
56	1	13	4.676	65.400	65.400	0.0	13.448	4.121	**
58	1	13	107.046	100.948	100.948	0.0	-10.423	-3.487	**
60	1	13	24.355	19.821	19.821	0.0	6.598	1.983	**
62	1	13	105.540	108.571	108.571	0.0	7.035	1.475	**
64	1	13	95.238	105.165	105.165	0.0	-3.027	-0.986	**
66	1	13	42.858	57.195	57.195	0.0	-14.208	-4.228	**
68	1	14	46.250	50.457	50.457	0.0	14.207	4.650	**
70	1	14	92.107	82.754	82.754	0.0	-10.247	-1.368	**
72	1	14	36.815	38.501	38.501	0.0	10.684	3.210	**
74	1	14	197.663	197.663	197.663	0.0	-11.669	-3.800	**
76	1	14	44.621	49.035	49.035	0.0	-4.415	-0.217	**
78	1	14	40.995	31.769	31.769	0.0	3.226	1.436	**
80	1	14	45.257	48.707	48.707	0.0	-8.115	-3.049	**
82	1	14	14.392	39.841	39.841	0.0	5.456	1.714	**
84	1	14	104.371	6.005	6.005	0.0	8.337	2.714	**
86	1	14	79.585	105.639	105.639	0.0	-1.268	-0.442	**
88	1	15	70.298	71.430	71.430	0.0	8.155	3.132	**
90	1	15	49.172	79.941	79.941	0.0	-9.643	-3.196	**
92	1	15	36.898	54.720	54.720	0.0	-5.548	-1.804	**
94	1	15	99.277	99.277	99.277	0.0	-2.379	-0.774	**
96	1	15	32.658	32.658	32.658	0.0	-0.809	-0.263	**
98	1	15	14.453	19.738	19.738	0.0	-5.285	-1.719	**



Table 2 (cont.)  
PAGE 20-8

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
0	1	1	30.974	36.353	-36.353	0.0	3.501	1.139
0	1	1	34.079	29.056	29.056	0.0	-4.571	2.511
0	1	1	35.087	31.058	41.688	0.0	-4.571	-1.486
0	1	1	35.927	32.278	-29.022	0.0	3.647	2.149
0	1	1	40.572	37.342	-17.522	0.0	-3.230	1.186
0	1	1	40.674	37.404	17.494	0.0	3.270	-1.971
0	1	1	55.074	54.804	58.823	0.0	0.270	1.057
0	1	1	176.668	185.023	-125.823	0.0	-8.355	0.076
0	1	1	187.423	197.423	125.823	0.0	-11.223	-3.682
0	1	1	197.423	197.423	39.023	0.0	0.001	0.130
0	1	1	33.520	36.952	-39.023	0.0	-3.402	1.106
0	1	1	132.422	130.588	15.838	0.0	-10.838	-3.375
0	1	1	132.422	137.632	-15.838	0.0	18.166	2.655
0	1	1	52.152	61.161	-15.838	0.0	0.091	0.091
0	1	1	13.664	14.050	-11.121	0.0	-0.386	0.119
0	1	1	40.008	34.895	34.895	0.0	-5.112	2.929
0	1	1	22.541	27.892	-27.892	0.0	5.351	-0.663
0	1	1	159.416	167.115	167.115	0.0	-7.699	1.740
0	1	1	64.078	64.704	-14.078	0.0	0.626	2.504
0	1	1	173.478	178.445	178.445	0.0	-4.967	0.060
0	1	1	122.084	132.862	-132.862	0.0	10.778	1.618
0	1	1	97.320	105.536	-105.536	0.0	8.216	-3.505
0	1	1	105.171	118.054	118.054	0.0	-12.883	2.701
0	1	1	19.875	16.374	16.374	0.0	3.501	-4.189
0	1	1	40.346	35.698	35.698	0.0	4.648	1.512
0	1	1	186.416	186.700	-214.397	0.0	-13.058	0.092
0	1	1	201.260	214.397	186.700	0.0	-4.246	4.246
0	1	1	61.688	58.264	-58.264	0.0	3.423	1.113
0	1	1	229.838	249.833	-249.833	0.0	13.595	-6.502
0	1	1	38.624	36.418	36.418	0.0	-2.206	0.718
0	1	1	56.854	72.696	-72.696	0.0	5.842	-1.900
0	1	1	25.585	24.882	-24.882	0.0	1.075	0.329
0	1	1	78.417	77.347	-77.347	0.0	1.075	0.348
0	1	1	41.238	41.878	-41.878	0.0	0.640	0.208
0	1	1	90.500	85.814	-85.814	0.0	4.686	-1.696
0	1	1	16.544	24.637	-24.637	0.0	8.091	-2.641
0	1	1	76.448	76.629	-76.629	0.0	0.181	0.069
0	1	1	133.216	137.634	-137.634	0.0	4.418	-1.437
0	1	1	76.356	76.617	-76.617	0.0	0.261	0.085
0	1	1	88.555	88.441	-88.441	0.0	0.114	0.089
0	1	1	57.106	56.230	-56.230	0.0	0.875	0.089
0	1	1	60.488	66.823	-66.823	0.0	6.335	-0.285
0	1	1	209.788	209.049	209.049	0.0	0.739	0.300
0	1	1	17.774	16.585	-16.585	0.0	1.190	0.280
0	1	1	43.023	38.821	-38.821	0.0	4.202	1.381
0	1	1	70.422	68.265	-68.265	0.0	2.157	0.786
0	1	1	94.901	97.689	-97.689	0.0	2.788	0.661
0	1	1	155.422	167.818	-167.818	0.0	-12.376	-3.887
0	1	1	80.282	76.414	-76.414	0.0	3.870	1.232
0	1	1	55.261	61.597	-61.597	0.0	-6.336	-1.684
0	1	1	78.078	71.655	-73.655	0.0	6.424	-1.499

HCLB H REFINEMENT - ALL OTHERS FIXED ANISOTROPIC - CYCLE 32(9-22-77)

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	*
14	1	N	40.715	43.480	-43.480	0.0	-2.765	-0.899	
15	1	N	52.129	79.689	79.689	0.0	3.440	1.121	*
18	1	N	57.709	43.104	-46.104	0.0	-8.398	-2.687	**
18	0	N	57.709	40.698	30.698	0.0	6.441	2.095	
12	1	N	59.435	70.631	16.631	0.0	-3.151	-1.038	
11	1	N	57.570	29.743	21.983	0.0	-7.724	-2.512	
11	1	N	15.145	17.521	-2.376	0.0	-8.373	-2.723	
15	1	N	20.922	37.508	15.508	0.0	0.207	0.563	
15	1	N	15.974	27.615	12.635	0.0	0.627	1.729	
15	1	N	30.193	17.920	-12.273	0.0	-0.236	-0.687	
11	1	N	32.522	18.881	-13.641	0.0	3.930	5.355	
11	1	N	19.081	18.985	-0.104	0.0	1.668	4.668	
11	1	N	65.074	92.695	27.621	0.0	2.412	0.784	
11	1	N	44.726	45.520	1.794	0.0	-0.258	-0.773	
11	1	N	129.587	129.707	-0.120	0.0	0.071	0.935	
11	1	N	139.397	124.176	15.221	0.0	-2.576	-0.888	*
11	1	N	34.156	33.225	0.931	0.0	-0.570	-1.601	**
11	1	N	15.899	26.800	10.901	0.0	4.525	1.222	
11	1	N	73.158	68.233	5.925	0.0	-3.263	-1.061	
11	1	N	67.171	70.880	-3.709	0.0	6.449	2.097	
11	1	N	43.975	47.278	-3.303	0.0	3.756	1.041	
11	1	N	134.262	140.719	-6.457	0.0	3.201	2.214	
11	1	N	75.680	79.476	-3.796	0.0	-2.786	-0.906	
11	1	N	209.664	206.463	3.201	0.0	7.479	2.497	
11	1	N	116.918	110.110	6.808	0.0	-1.614	-0.525	
11	1	N	40.100	42.885	-2.785	0.0	-0.970	-1.786	
11	1	N	50.494	55.253	-4.759	0.0	2.057	0.385	*
11	1	N	29.138	20.459	8.679	0.0	1.356	0.328	*
11	1	N	79.923	81.577	-1.654	0.0	-1.817	-1.672	*
11	1	N	95.545	90.055	5.490	0.0	2.412	1.104	
11	1	N	37.640	38.617	-0.977	0.0	-0.328	-0.440	
11	1	N	99.604	93.617	5.987	0.0	1.356	0.478	
11	1	N	16.606	17.759	-1.153	0.0	0.4134	1.300	
11	1	N	16.606	19.681	-3.075	0.0	-0.243	-0.686	
11	1	N	73.773	74.731	-0.958	0.0	-1.686	-1.087	
11	1	N	14.053	19.682	-5.629	0.0	5.095	1.657	
11	1	N	46.681	41.529	5.152	0.0	1.104	1.104	
11	1	N	59.935	19.181	40.754	0.0	-0.440	-5.078	
11	1	N	187.093	50.307	136.786	0.0	6.449	2.097	
11	1	N	183.464	183.607	-0.143	0.0	0.4134	1.300	
11	1	N	221.350	184.817	36.533	0.0	-0.243	-0.686	
11	1	N	344.954	198.723	146.231	0.0	1.104	1.104	
11	1	N	22.581	21.617	0.964	0.0	0.4134	1.300	
11	1	N	41.369	237.235	-195.866	0.0	-0.243	-0.686	
11	1	N	79.984	80.703	-0.719	0.0	-1.686	-1.087	
11	1	N	113.135	115.021	-1.886	0.0	5.095	1.657	
11	1	N	62.272	57.177	5.095	0.0	1.104	1.104	

Table 2 (cont.)  
PAGE 810

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
11	2	5	53.692	53.518	53.518	0.0	0.174	0.057	
11	2	5	53.476	53.342	53.342	0.0	-0.134	-0.032	
11	2	5	55.048	52.924	52.924	0.0	-2.124	-0.610	
15	5	5	44.821	43.547	43.547	0.0	-1.274	-0.091	
15	5	5	77.802	77.136	77.136	0.0	-0.666	-0.200	
17	2	5	12.511	12.877	12.877	0.0	0.366	0.060	
17	2	5	11.163	11.859	11.859	0.0	-0.696	-0.214	**
19	2	5	50.002	40.064	40.064	0.0	-9.938	-3.232	
19	2	5	90.004	94.860	94.860	0.0	4.856	1.257	
19	2	5	85.149	87.138	87.138	0.0	1.989	0.088	
19	2	5	56.577	66.307	66.307	0.0	9.730	1.447	**
22	4	5	17.240	16.628	16.628	0.0	-0.612	-0.194	
22	4	5	53.180	6.448	6.448	0.0	-46.732	-14.447	**
22	4	5	14.115	9.343	9.343	0.0	-4.772	-1.447	**
22	4	5	57.629	59.604	59.604	0.0	1.975	0.642	**
22	4	5	12.024	13.638	13.638	0.0	1.614	0.590	**
22	4	5	27.123	25.945	25.945	0.0	-1.178	-0.383	
22	4	5	13.524	13.491	13.491	0.0	-0.033	-0.010	
22	4	5	13.660	14.037	14.037	0.0	0.376	0.085	**
22	4	5	5.781	5.520	5.520	0.0	-0.261	-0.085	**
22	4	5	53.938	53.485	53.485	0.0	-0.453	-0.147	
22	4	5	15.403	15.642	15.642	0.0	0.239	0.006	**
22	4	5	3.475	19.384	19.384	0.0	15.909	5.173	**
22	4	5	50.094	48.466	48.466	0.0	-1.628	-0.530	
22	4	5	75.526	72.814	72.814	0.0	-2.712	-0.882	
22	4	5	53.016	52.610	52.610	0.0	-0.406	-0.132	
22	4	5	29.522	26.344	26.344	0.0	-3.178	-1.016	**
22	4	5	45.789	44.328	44.328	0.0	-1.461	-0.475	
22	4	5	196.416	188.983	188.983	0.0	-7.433	-2.455	**
22	4	5	39.977	37.123	37.123	0.0	-2.854	-0.928	**
22	4	5	13.408	4.182	4.182	0.0	-9.226	-3.000	**
22	4	5	15.323	153.998	153.998	0.0	138.675	47.382	**
22	4	5	18.444	135.173	135.173	0.0	116.729	39.287	**
22	4	5	12.485	12.435	12.435	0.0	-0.050	-0.016	**
22	4	5	52.432	48.237	48.237	0.0	-4.195	-1.352	
22	4	5	88.934	84.658	84.658	0.0	-4.276	-1.420	
22	4	5	150.049	127.201	127.201	0.0	-22.848	-7.647	**
22	4	5	144.900	137.925	137.925	0.0	-6.975	-2.325	
22	4	5	99.789	102.234	102.234	0.0	2.445	0.820	
22	4	5	100.389	170.907	170.907	0.0	70.518	23.082	**
22	4	5	61.318	64.321	64.321	0.0	3.003	1.007	
22	4	5	20.880	19.366	19.366	0.0	-1.514	-0.492	
22	4	5	37.454	90.352	90.352	0.0	52.898	18.005	**
22	4	5	32.459	31.134	31.134	0.0	-1.325	-0.414	
22	4	5	32.976	89.737	89.737	0.0	56.761	19.230	**
22	4	5	78.269	59.600	59.600	0.0	-18.669	-6.230	**
22	4	5	70.420	55.955	55.955	0.0	-14.465	-4.954	**
22	4	5	104.305	112.819	112.819	0.0	7.486	2.487	
22	4	5	114.325	101.498	101.498	0.0	-12.827	-4.277	**
22	4	5	130.077	116.113	116.113	0.0	-13.964	-4.880	**
22	4	5	129.702	126.702	126.702	0.0	6.999	2.331	**
22	4	5	24.571	13.416	13.416	0.0	-11.155	-3.627	**

Table 2 (cont)  
PAGE 211

H	K	L	F(OBS)	F(CALC)	A(CALC)	R(CALC)	DELTA F	DELTA/SIGMA
0	0	0	131.972	96.338	0.0	0.0	5.634	1.832
0	0	0	132.808	136.337	0.0	0.0	6.529	2.132
0	0	0	135.058	131.345	0.0	0.0	1.713	0.557
0	0	0	135.163	152.541	0.0	0.0	2.621	0.852
0	0	0	111.378	77.437	0.0	0.0	1.902	0.618
0	0	0	111.378	11.620	0.0	0.0	9.475	3.081
0	0	0	111.378	25.952	0.0	0.0	-4.739	-0.672
0	0	0	111.378	46.707	0.0	0.0	-2.058	-0.672
0	0	0	111.378	41.707	0.0	0.0	3.518	1.144
0	0	0	111.378	34.085	0.0	0.0	3.487	1.134
0	0	0	111.378	27.504	0.0	0.0	-3.302	-0.74
0	0	0	111.378	27.504	0.0	0.0	-0.993	-0.313
0	0	0	111.378	3.044	0.0	0.0	5.531	1.818
0	0	0	111.378	0.447	0.0	0.0	-0.519	-0.170
0	0	0	186.457	186.457	0.0	0.0	0.000	0.000
0	0	0	22.945	22.945	0.0	0.0	0.000	0.000
0	0	0	194.932	194.932	0.0	0.0	0.000	0.000
0	0	0	194.932	29.479	0.0	0.0	1.453	0.359
0	0	0	24.632	30.494	0.0	0.0	1.402	0.359
0	0	0	20.245	21.015	0.0	0.0	-1.566	-0.566
0	0	0	40.777	34.205	0.0	0.0	8.572	2.676
0	0	0	67.561	64.953	0.0	0.0	2.608	0.848
0	0	0	67.561	66.773	0.0	0.0	0.788	0.237
0	0	0	25.278	35.470	0.0	0.0	-10.192	-3.314
0	0	0	137.429	134.501	0.0	0.0	2.928	0.952
0	0	0	119.716	147.732	0.0	0.0	-7.016	-2.296
0	0	0	44.805	121.322	0.0	0.0	-76.517	-22.711
0	0	0	55.901	48.068	0.0	0.0	7.833	2.296
0	0	0	45.621	59.261	0.0	0.0	-13.640	-3.919
0	0	0	45.621	47.989	0.0	0.0	-2.368	-0.667
0	0	0	8.764	4.352	0.0	0.0	4.412	1.261
0	0	0	54.907	56.907	0.0	0.0	-1.999	-0.571
0	0	0	72.881	78.025	0.0	0.0	-5.144	-1.473
0	0	0	45.820	46.303	0.0	0.0	-0.483	-0.137
0	0	0	77.463	72.709	0.0	0.0	4.754	1.346
0	0	0	131.309	132.588	0.0	0.0	-1.279	-0.366
0	0	0	77.187	70.248	0.0	0.0	6.939	2.056
0	0	0	50.156	46.029	0.0	0.0	4.127	1.174
0	0	0	48.834	48.794	0.0	0.0	0.040	0.011
0	0	0	11.870	15.446	0.0	0.0	-3.576	-1.061
0	0	0	30.075	8.489	0.0	0.0	21.586	6.105
0	0	0	49.112	25.997	0.0	0.0	23.115	6.686
0	0	0	99.112	48.214	0.0	0.0	50.898	14.602
0	0	0	15.038	101.505	0.0	0.0	-86.467	-24.429
0	0	0	18.937	34.377	0.0	0.0	-15.440	-4.557
0	0	0	18.937	20.535	0.0	0.0	8.402	2.459
0	0	0	18.937	25.459	0.0	0.0	-6.522	-1.917
0	0	0	37.022	10.402	0.0	0.0	26.620	7.743
0	0	0	37.117	31.065	0.0	0.0	6.052	1.743
0	0	0	11.563	15.005	0.0	0.0	-3.442	-1.008
0	0	0	41.330	40.477	0.0	0.0	0.853	0.247

Table 2 (cont)  
PAGE#12

HCLR F REFINEMENT -ALL OTHERS FIXED ANISOTROPIC- CYCLE 32(9-22-77)

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
1	1	1	18.286	118.121	118.121	0.0	-0.034	-0.011	
1	1	1	18.286	97.496	97.496	0.0	0.241	0.241	
1	1	1	18.286	70.226	-30.226	0.0	-1.566	-0.509	
1	1	1	18.286	120.826	176.826	0.0	-4.068	-1.323	
1	1	1	17.070	12.994	132.994	0.0	-2.894	-0.938	
1	1	1	17.070	28.265	12.121	0.0	-1.546	-0.503	
1	1	1	17.070	4.646	25.985	0.0	-8.980	-2.920	
1	1	1	18.286	8.646	-43.646	0.0	12.450	4.052	
1	1	1	18.286	8.322	8.422	0.0	9.907	3.157	
1	1	1	17.070	2.922	8.399	0.0	5.967	0.942	
1	1	1	17.070	40.122	2.922	0.0	1.648	1.648	
1	1	1	17.070	55.303	40.164	0.0	-3.622	-1.061	
1	1	1	17.070	32.368	55.368	0.0	-1.849	-0.601	
1	1	1	195.180	207.575	32.618	0.0	-2.937	-0.937	
1	1	1	22.264	20.315	207.575	0.0	-12.373	-4.024	
1	1	1	99.045	37.477	20.315	0.0	-1.949	-0.634	
1	1	1	43.483	8.307	-37.043	0.0	-3.643	-1.185	
1	1	1	21.618	155.607	8.307	0.0	6.046	1.966	
1	1	1	149.484	186.671	155.607	0.0	-13.315	-4.330	
1	1	1	85.212	18.447	-18.671	0.0	-1.989	-0.674	
1	1	1	131.555	138.820	18.447	0.0	-11.175	-3.634	
1	1	1	109.199	107.757	-107.757	0.0	2.362	2.362	
1	1	1	32.781	9.069	19.075	0.0	1.446	0.470	
1	1	1	30.875	18.728	18.728	0.0	14.166	4.607	
1	1	1	106.647	113.648	-22.728	0.0	-8.097	-2.633	
1	1	1	41.515	40.154	113.648	0.0	-7.902	-2.277	
1	1	1	60.827	54.553	-40.354	0.0	1.760	0.442	
1	1	1	97.131	68.063	-64.553	0.0	-3.726	-1.212	
1	1	1	23.648	28.617	-68.063	0.0	-0.872	-0.284	
1	1	1	45.205	41.219	-28.219	0.0	4.969	1.616	
1	1	1	66.577	66.755	-41.219	0.0	-3.986	-1.296	
1	1	1	130.594	140.732	-66.577	0.0	-0.188	-0.061	
1	1	1	27.031	27.923	140.732	0.0	-10.008	-3.254	
1	1	1	40.521	38.443	-38.443	0.0	0.323	0.300	
1	1	1	122.084	125.911	-38.443	0.0	-3.069	-0.673	
1	1	1	150.002	52.259	52.259	0.0	-3.927	-1.244	
1	1	1	7.934	11.250	11.250	0.0	-3.372	-0.734	
1	1	1	35.764	45.112	-45.112	0.0	3.706	1.078	
1	1	1	120.300	252.914	45.112	0.0	-29.545	-9.607	
1	1	1	120.329	124.722	124.722	0.0	-2.527	-0.813	
1	1	1	51.232	56.806	56.806	0.0	-5.574	-1.671	
1	1	1	212.678	238.884	238.884	0.0	-27.204	-8.113	
1	1	1	99.856	97.503	-97.503	0.0	17.646	5.222	
1	1	1	11.101	9.713	9.713	0.0	-1.489	-0.487	
1	1	1	78.078	86.557	-86.557	0.0	1.479	0.452	
1	1	1	55.783	57.935	57.935	0.0	-2.152	-0.700	
1	1	1	22.756	9.077	9.077	0.0	13.679	4.157	
1	1	1	198.564	198.977	198.977	0.0	-0.383	-0.128	
1	1	1	13.131	16.687	16.687	0.0	-3.556	-1.157	

Table 2 (cont)  
PAGE#13

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
2	4	1	261.788	291.566	-91.566	0.00	-29.778	-9.683	*
4	6	1	250.774	289.506	-89.506	0.00	-5.656	-1.839	*
0	0	0	250.774	286.599	-86.599	0.00	-25.825	-8.398	*
0	0	0	75.118	84.984	9.866	0.00	-4.932	-1.601	
0	0	0	234.680	242.480	8.800	0.00	-7.599	-2.471	
0	0	0	121.570	122.775	1.205	0.00	-6.203	-2.030	
0	0	0	93.823	92.529	-1.294	0.00	0.421	0.421	
0	0	0	92.371	97.570	5.199	0.00	-1.259	-1.863	
0	0	0	23.371	31.643	8.272	0.00	-4.854	-1.578	
0	0	0	11.378	20.852	9.474	0.00	-3.690	-3.292	**
0	0	0	9.051	45.852	36.801	0.00	8.517	2.770	**
0	0	0	8.918	101.025	92.107	0.00	-2.044	-0.665	*
0	0	0	12.157	101.025	88.868	0.00	-5.123	-1.666	*
0	0	0	84.874	81.310	-3.564	0.00	4.847	1.576	
0	0	0	91.855	91.557	-0.298	0.00	2.951	0.950	
0	0	0	62.210	61.235	-0.975	0.00	-1.698	-0.552	
0	0	0	49.172	53.375	4.203	0.00	-0.790	-0.257	
0	0	0	37.025	32.322	-4.703	0.00	-4.163	-1.354	
0	0	0	101.757	102.202	0.445	0.00	-0.449	-0.264	
0	0	0	55.378	96.392	41.014	0.00	-1.248	-0.406	
0	0	0	34.905	34.400	-0.505	0.00	4.252	1.610	
0	0	0	53.725	49.401	-5.324	0.00	0.754	0.258	
0	0	0	30.413	96.512	66.100	0.00	-4.533	-1.376	
0	0	0	25.124	28.777	3.653	0.00	-4.503	-1.594	
0	0	0	39.977	43.174	3.197	0.00	2.347	0.763	
0	0	0	113.904	118.541	4.637	0.00	-4.637	-1.027	
0	0	0	175.959	175.959	0.000	0.00	0.000	0.000	
0	0	0	31.028	29.301	-1.727	0.00	-4.637	-1.508	
0	0	0	16.421	22.964	6.543	0.00	1.728	0.286	
0	0	0	26.938	6.095	-20.843	0.00	-10.729	-0.562	**
0	0	0	79.895	70.945	-8.950	0.00	10.412	3.386	**
0	0	0	80.938	30.511	-50.427	0.00	-4.347	-2.910	**
0	0	0	4.520	82.773	78.253	0.00	-4.156	-1.352	**
0	0	0	53.723	12.533	-41.190	0.00	-2.435	-0.922	**
0	0	0	64.066	55.966	-8.100	0.00	7.430	1.186	
0	0	0	113.955	113.955	0.000	0.00	0.000	0.000	
0	0	0	119.122	119.912	0.790	0.00	0.790	0.016	
0	0	0	14.014	4.199	-9.815	0.00	-2.886	-0.257	**
0	0	0	103.571	24.950	-78.621	0.00	4.663	1.516	
0	0	0	43.022	110.216	67.194	0.00	-0.044	-2.161	
0	0	0	28.445	43.096	14.651	0.00	-3.289	-0.914	
0	0	0	91.353	30.744	-60.609	0.00	-1.048	-0.748	
0	0	0	66.069	89.278	23.209	0.00	-3.528	-0.678	*
0	0	0	11.132	68.167	57.035	0.00	-1.528	-0.497	**
0	0	0	14.509	11.766	-3.743	0.00	-0.160	-0.206	**
0	0	0	119.778	111.191	-8.587	0.00	8.587	2.792	

Table 1 (cont)  
PAGE 14

HCLB K REFINEMENT - ALL OTHERS FIXED ANISOTROPIC- CYCLE 32(9-22-77)										STRUCTURE FACTORS	
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA			
-15	0	3	55.753	57.825	-57.825	0.0	-2.072	-0.674			
-18	0	3	110.700	100.612	-100.612	0.0	10.076	3.342			
-20	0	3	86.871	84.871	-84.871	0.0	-3.164	-1.029			
-1	1	4	104.377	104.792	-106.792	0.0	9.541	3.103			
-3	0	4	95.328	95.335	55.335	0.0	1.302	0.423			
-3	0	4	105.281	95.330	68.530	0.0	2.998	0.575			
-3	0	4	105.519	173.233	173.233	0.0	-5.047	-0.666			
-5	0	4	23.517	30.541	-20.541	0.0	3.076	1.000			
-7	0	4	66.652	171.564	-91.464	0.0	5.189	1.687			
-7	0	4	49.855	153.731	-110.591	0.0	-4.590	-1.493			
-0	0	4	19.743	18.918	-32.137	0.0	-3.232	-1.054			
-11	0	4	31.490	30.429	-18.918	0.0	0.885	0.268			
-13	0	4	29.820	26.263	-30.423	0.0	1.066	0.347			
-15	0	4	55.420	57.512	59.203	0.0	3.626	1.179			
-17	0	4	45.420	44.077	-37.518	0.0	-1.085	-0.353			
-17	0	4	33.273	29.008	-49.076	0.0	1.344	0.437			
-19	0	4	88.872	80.271	-60.098	0.0	4.265	1.387			
-19	0	4	105.281	19.443	19.443	0.0	8.601	2.797			
-1	0	5	97.702	88.720	-88.720	0.0	-0.162	-0.053	*	**	
-2	0	5	125.803	125.837	125.837	0.0	0.963	0.320			
-2	0	5	156.318	198.510	-198.510	0.0	3.966	1.290			
-4	0	5	260.927	255.101	-225.101	0.0	-2.192	-0.713			
-4	0	5	108.030	106.755	-106.755	0.0	5.236	1.695			
-5	0	5	47.173	51.433	-51.433	0.0	1.275	0.415			
-5	0	5	33.150	25.943	-25.943	0.0	-4.262	-1.386			
-8	0	5	151.723	163.084	-163.084	0.0	7.307	2.344			
-10	0	5	106.185	101.172	-101.172	0.0	-1.431	-0.443			
-12	0	5	59.597	58.969	-58.969	0.0	5.013	1.630			
-12	0	5	4.828	13.613	-13.613	0.0	0.528	0.204			
-14	0	5	22.110	19.855	-19.855	0.0	-5.285	-2.857	*	**	
-16	0	5	87.150	85.157	85.157	0.0	2.233	0.733			
-16	0	5	17.375	7.5055	-7.5055	0.0	1.953	0.648			
-18	0	5	20.265	23.707	-23.707	0.0	-0.344	-0.119	*	**	
-18	0	5	59.966	60.434	-60.434	0.0	-3.441	-1.119	*	**	
-1	0	6	18.881	15.316	-15.316	0.0	-3.569	-0.152			
-3	0	6	20.481	29.320	29.320	0.0	7.830	1.160			
-5	0	6	19.835	23.972	23.972	0.0	-1.177	-0.375			
-5	0	6	62.026	59.169	-59.169	0.0	-1.285	-0.429			
-7	0	6	166.705	160.518	-160.518	0.0	2.487	0.929			
-7	0	6	49.787	67.107	67.107	0.0	-0.311	-0.102			
-9	0	6	24.694	50.756	-50.756	0.0	-0.246	-0.085			
-11	0	6	26.293	29.737	-29.737	0.0	-5.043	-1.715			
-11	0	6	25.801	25.681	-25.681	0.0	0.119	0.040			
-13	0	6	13.162	19.694	19.694	0.0	6.107	1.999			
-13	0	6	57.838	15.335	15.335	0.0	-2.107	-0.713	*	**	
-17	0	6	22.602	68.641	68.641	0.0	-0.803	-0.261	*	**	
-17	0	6	68.914	28.831	28.831	0.0	-0.329	-0.107	*	**	
-17	0	6	40.469	69.841	69.841	0.0	-0.936	-0.304	*	**	
-0	0	7	45.851	41.327	-41.327	0.0	-0.858	-0.279	*	**	
-0	0	7		46.491	-46.491	0.0	-0.441	-0.120	*	**	



Table 2 (cont.)  
PAGE 315

HCLB H REFINEMENT - ALL OTHERS FIXED ANISOTROPIC- CYCLE 32(9-22-77)									
H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
2	3	7	123.379	127.338	-127.338	0.0	-3.963	-1.289	
4	3	7	130.940	120.032	-120.032	0.0	10.908	3.547	
4	3	7	179.185	173.702	-173.702	0.0	5.483	1.783	
0	3	7	110.152	109.475	-109.475	0.0	0.677	0.220	
0	3	7	67.500	65.547	-65.547	0.0	1.953	0.803	
0	3	7	94.254	91.427	-91.427	0.0	2.827	0.419	
0	3	7	92.716	89.411	-89.411	0.0	3.305	0.786	
0	3	7	89.411	81.308	-81.308	0.0	8.103	2.710	
1	3	7	119.562	117.144	-117.144	0.0	2.418	0.786	
1	3	7	44.897	44.897	0.0	0.0	0.0	0.0	
1	3	7	69.099	70.637	-70.637	0.0	-3.538	-1.171	
1	3	7	151.944	149.941	-149.941	0.0	2.003	-0.500	
1	3	7	51.816	47.677	-47.677	0.0	4.140	1.346	
1	3	7	24.171	21.063	-21.063	0.0	3.108	1.011	
1	3	7	77.525	76.692	-76.692	0.0	0.833	0.270	
3	3	8	54.369	60.515	-60.515	0.0	6.147	-1.999	
3	3	8	73.835	67.794	-67.794	0.0	6.041	1.964	
3	3	8	37.117	27.136	-27.136	0.0	9.981	3.246	
3	3	8	71.282	75.647	-75.647	0.0	-4.365	-1.419	
5	3	8	155.572	152.889	-152.889	0.0	2.684	0.873	
7	3	8	34.473	31.260	-31.260	0.0	3.214	1.059	
7	3	8	33.704	32.493	-32.493	0.0	1.211	0.419	
7	3	8	32.255	27.492	-27.492	0.0	4.763	1.587	
9	3	8	91.027	88.262	-88.262	0.0	2.765	0.898	
9	3	8	33.027	28.491	-28.491	0.0	4.536	1.475	
9	3	8	86.258	80.657	-80.657	0.0	5.601	1.821	
9	3	8	14.361	2.101	-2.101	0.0	12.260	3.987	
9	3	8	58.520	56.666	-56.666	0.0	1.854	0.603	
9	3	8	43.331	44.778	-44.778	0.0	-1.447	-0.432	
9	3	8	30.025	35.511	-35.511	0.0	5.486	1.783	
9	3	8	106.023	105.044	-105.044	0.0	0.978	0.338	
9	3	8	156.033	160.938	-160.938	0.0	-4.905	-1.505	
9	3	8	21.220	22.289	-22.289	0.0	-1.069	-0.328	
9	3	8	147.044	144.345	-144.345	0.0	2.692	0.881	
9	3	8	91.928	94.131	-94.131	0.0	-2.203	-0.700	
9	3	8	89.825	88.377	-88.377	0.0	1.453	0.471	
9	3	8	98.347	94.209	-94.209	0.0	4.134	1.344	
9	3	8	75.927	75.526	-75.526	0.0	0.401	0.150	
9	3	8	154.855	151.609	-151.609	0.0	3.247	1.059	
9	3	8	166.151	162.745	-162.745	0.0	3.406	1.124	
9	3	8	11.685	16.520	-16.520	0.0	-4.835	-1.551	
9	3	8	73.835	74.583	-74.583	0.0	-0.748	-0.229	
9	3	8	71.685	68.535	-68.535	0.0	3.154	1.059	
9	3	8	80.652	78.499	-78.499	0.0	2.153	0.715	
9	3	8	23.944	16.395	-16.395	0.0	7.549	2.439	
9	3	8	13.315	10.981	-10.981	0.0	2.334	0.811	
9	3	8	43.052	42.866	-42.866	0.0	0.186	0.062	
9	3	8	130.088	130.601	-130.601	0.0	-0.514	-0.171	
9	3	8	130.049	130.601	-130.601	0.0	-0.552	-0.180	
9	3	8	21.987	23.772	-23.772	0.0	-1.785	-0.580	
9	3	8	90.873	86.769	-86.769	0.0	4.103	1.354	

Table 2 (cont)  
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H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
1	0	0	33.827	38.173	-38.173	0.0	-4.347	1.413	*
1	0	0	17.897	34.147	-34.147	0.0	-16.249	-15.284	**
1	0	0	115.294	104.635	104.635	0.0	1.201	0.391	
1	0	0	24.767	104.635	-13.147	0.0	11.333	1.344	
1	0	0	37.979	78.147	-38.207	0.0	5.330	3.705	
1	0	0	94.520	77.320	-79.320	0.0	1.374	-0.074	
1	0	0	64.917	68.861	-77.861	0.0	-1.320	1.429	
1	0	0	55.950	47.817	-47.817	0.0	-2.552	-1.224	
1	0	0	16.192	7.192	-47.192	0.0	7.780	-2.550	**
1	0	0	58.520	55.442	-55.442	0.0	9.780	3.180	
1	0	0	47.091	40.492	-40.492	0.0	-3.341	-2.251	
1	0	0	41.299	67.492	-67.492	0.0	5.021	1.088	
1	0	0	72.542	56.776	-57.422	0.0	5.051	1.643	
1	0	0	104.432	105.130	105.130	0.0	5.771	1.877	
1	0	0	46.435	61.432	-61.432	0.0	-0.699	-0.227	
1	0	0	54.707	50.822	-50.822	0.0	-4.742	-1.674	
1	0	0	83.860	79.088	-79.088	0.0	-2.472	-0.804	
1	0	0	22.049	7.085	-7.085	0.0	4.761	1.548	
1	0	0	34.592	94.003	-94.003	0.0	14.063	4.573	
1	0	0	55.850	60.122	-60.122	0.0	5.277	1.866	
1	0	0	56.890	53.523	-53.523	0.0	3.377	1.098	*
1	0	0	8.118	19.594	-19.594	0.0	3.377	1.098	**
1	0	0	22.101	94.121	-94.121	0.0	3.377	1.098	
1	0	0	57.875	55.791	-55.791	0.0	-2.020	-0.657	
1	0	0	94.038	95.617	-95.617	0.0	-1.578	-0.678	
1	0	0	78.453	92.946	-92.946	0.0	-2.084	-0.513	
1	0	0	27.799	83.221	-83.221	0.0	-2.084	-0.513	
1	0	0	86.105	80.328	-80.328	0.0	-5.022	-1.637	
1	0	0	121.428	128.655	-128.655	0.0	5.756	1.885	
1	0	0	51.828	55.756	-55.756	0.0	-7.227	-2.360	
1	0	0	45.525	44.750	-44.750	0.0	-3.058	-1.254	
1	0	0	50.320	36.088	-36.088	0.0	-1.715	-0.582	
1	0	0	11.586	5.721	-5.721	0.0	8.528	2.912	
1	0	0	36.717	41.257	-41.257	0.0	-0.588	-0.191	*
1	0	0	37.240	43.822	-43.822	0.0	-4.355	-2.262	**
1	0	0	42.420	36.521	-36.521	0.0	-4.355	-2.262	
1	0	0	20.450	8.707	-8.707	0.0	12.373	1.917	*
1	0	0	74.911	76.994	-76.994	0.0	-2.079	-0.614	**
1	0	0	18.933	16.385	-16.385	0.0	-2.079	-0.614	*
1	0	0	78.140	79.059	-79.059	0.0	-0.710	-0.239	**
1	0	0	93.425	96.424	-96.424	0.0	-0.710	-0.239	*
1	0	0	53.341	21.021	-21.021	0.0	11.739	0.887	
1	0	0	32.721	348.182	-348.182	0.0	11.739	3.804	*
1	0	0	44.744	51.334	-51.334	0.0	-24.522	-2.844	*
1	0	0					-0.590	-2.143	

Table 2 (cont)  
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HCLB F REFINEMENT - ALL OTHERS FIXED ANISOTROPIC - CYCLE 32(9-22-77)				STRUCTURE FACTORS				
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-5	-4	0	44.528	48.879	-48.879	0.0	-4.351	-1.415
-8	-4	0	74.329	74.438	-74.438	0.0	-0.109	-0.016
-10	-4	0	74.783	74.783	0.0	0.0	0.0	-1.389
-12	-4	0	51.012	51.022	54.022	0.0	3.010	0.006
-14	-4	0	21.758	21.906	-21.906	0.0	-9.255	0.002
-18	-4	0	45.095	45.046	-3.849	0.0	-3.081	0.002
-1	-4	0	130.041	130.817	-48.779	0.0	-3.698	0.409
-3	-4	0	20.176	20.725	-136.817	0.0	-1.258	0.202
-5	-4	0	58.093	58.398	-38.255	0.0	-1.756	0.581
-7	-4	0	134.326	134.433	-54.398	0.0	-0.918	0.299
-9	-4	0	77.741	78.433	-68.593	0.0	-0.167	0.054
-11	-4	0	44.282	48.242	-198.434	0.0	-6.108	-1.986
-13	-4	0	56.486	54.572	-78.222	0.0	-2.481	-0.807
-15	-4	0	193.874	209.523	-48.542	0.0	-4.260	-1.385
-17	-4	0	45.408	44.573	-64.826	0.0	-0.150	-0.062
-19	-4	0	103.756	106.873	-249.523	0.0	-16.705	-5.415
-21	-4	0	21.342	20.790	-46.573	0.0	-0.444	-0.151
-23	-4	0	54.123	53.897	-20.790	0.0	-0.251	-0.179
-25	-4	0	30.450	42.201	-42.201	0.0	-0.226	-0.073
-27	-4	0	31.240	14.001	14.001	0.0	0.222	0.027
-29	-4	0	56.454	36.149	-29.572	0.0	-7.688	-2.494
-31	-4	0	32.320	66.438	66.438	0.0	5.488	1.785
-33	-4	0	43.658	47.735	-31.672	0.0	-0.267	-0.005
-35	-4	0	38.470	41.610	47.735	0.0	-4.077	-1.313
-37	-4	0	18.820	16.769	-16.769	0.0	-3.150	-1.021
-39	-4	0	89.572	85.755	-85.755	0.0	-2.051	-0.667
-41	-4	0	77.187	76.706	-76.706	0.0	-0.441	-0.1274
-43	-4	0	20.235	15.875	-15.875	0.0	-4.781	-1.418
-45	-4	0	74.357	58.045	-58.045	0.0	-11.700	-3.785
-47	-4	0	34.811	75.251	75.251	0.0	4.770	0.291
-49	-4	0	79.278	39.590	-39.590	0.0	-4.700	-1.554
-51	-4	0	26.600	73.420	-73.420	0.0	-5.519	-1.905
-53	-4	0	21.741	21.752	-21.752	0.0	-0.011	-0.027
-55	-4	0	73.589	75.158	-75.158	0.0	-1.569	-0.503
-57	-4	0	44.129	15.859	-15.859	0.0	-1.578	-0.510
-59	-4	0	107.750	46.600	-46.600	0.0	-4.471	-1.553
-61	-4	0	209.480	16.063	-16.063	0.0	-20.066	-6.821
-63	-4	0	56.823	211.186	-211.186	0.0	-11.706	-4.255
-65	-4	0	132.478	71.189	-71.189	0.0	-4.366	-1.525
-67	-4	0	52.316	132.516	-132.516	0.0	-4.038	-1.412
-69	-4	0	238.603	63.109	-63.109	0.0	-2.207	-0.712
-71	-4	0	44.067	243.542	-243.542	0.0	-7.739	-2.387
-73	-4	0	43.114	45.967	-45.967	0.0	-1.900	-0.618
-75	-4	0	125.847	40.435	-40.435	0.0	-2.678	-0.971
-77	-4	0	138.905	108.198	-108.198	0.0	-0.745	-0.274
-79	-4	0		141.085	-141.085	0.0	-2.180	-0.709

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Table 2 (cont.)  
PAGE 2

HCLB F REFINEMENT - ALL STARS FIXED ANISOTROPIC - CYCLE 32(9-22-77)				STRUCTURE FACTORS				
M	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-1	4	4	56.307	56.234	-0.073	0.0	-1.927	-0.627
-1	4	4	32.616	32.621	0.005	0.0	4.226	4.226
-1	5	4	30.656	30.784	0.128	0.0	-0.042	-0.042
-1	5	4	42.850	42.729	-0.121	0.0	1.168	1.168
-1	7	4	31.717	31.703	-0.014	0.0	-0.548	-0.548
-1	7	4	35.710	35.692	-0.018	0.0	-0.891	-0.891
-1	7	4	31.753	31.715	-0.038	0.0	1.075	1.075
0	0	4	114.470	114.427	-0.043	0.0	-2.135	-2.135
2	2	4	14.175	14.427	0.252	0.0	0.240	0.240
-2	4	4	167.635	167.997	0.362	0.0	0.058	0.058
4	4	4	174.518	168.610	-5.908	0.0	-0.220	-0.220
4	4	4	9.901	164.807	154.906	0.0	1.857	1.857
4	4	4	16.707	96.100	79.393	0.0	-1.040	-1.040
4	4	4	17.897	11.335	-6.562	0.0	-0.856	-0.856
4	4	4	102.580	14.084	-88.496	0.0	1.240	1.240
8	8	4	30.292	103.077	72.785	0.0	-0.129	-0.129
-10	4	4	38.216	47.385	9.169	0.0	-1.129	-1.129
-10	4	4	11.071	4.385	-6.686	0.0	-9.069	-9.069
-12	4	4	34.042	28.572	-5.470	0.0	1.166	1.166
-12	4	4	75.649	74.572	-1.077	0.0	1.778	1.778
-14	4	4	72.051	70.516	-1.535	0.0	0.357	0.357
-14	4	4	45.635	45.820	0.185	0.0	0.466	0.466
-14	4	4	14.452	17.442	2.990	0.0	-1.361	-1.361
-16	4	4	76.510	77.652	1.142	0.0	-0.972	-0.972
-18	4	4	21.126	18.851	-2.275	0.0	-0.371	-0.371
-18	4	4	25.525	17.954	-7.571	0.0	0.740	0.740
-18	4	4	32.657	32.958	0.301	0.0	2.478	2.478
3	3	4	112.724	128.826	16.102	0.0	0.026	0.026
-5	4	4	15.161	96.308	81.147	0.0	1.268	1.268
-5	4	4	52.052	57.754	5.702	0.0	-0.152	-0.152
-7	4	4	29.390	33.585	4.195	0.0	1.851	1.851
-7	4	4	42.229	36.836	-5.393	0.0	-0.361	-0.361
-7	4	4	42.529	42.436	-0.093	0.0	2.081	2.081
9	4	4	36.840	36.450	-0.390	0.0	0.124	0.124
11	4	4	201.700	196.832	-4.868	0.0	1.583	1.583
-11	4	4	175.038	173.335	-1.703	0.0	0.165	0.165
-15	4	4	141.519	127.394	-14.125	0.0	0.254	0.254
-15	4	4	47.327	39.832	-7.495	0.0	2.437	2.437
-17	4	4	32.381	36.694	4.313	0.0	-1.402	-1.402
-17	4	4	78.078	90.219	12.141	0.0	-1.112	-1.112
0	4	4	76.268	83.133	6.865	0.0	0.584	0.584
-2	4	4	41.668	37.821	-3.847	0.0	-0.501	-0.501
-4	4	4	32.652	55.192	22.540	0.0	1.165	1.165
-4	4	4	74.849	69.827	-4.922	0.0	-0.170	-0.170
6	4	4	113.873	70.761	-42.112	0.0	1.422	1.422
6	4	4	50.002	114.050	64.048	0.0	-1.184	-1.184
10	4	4	26.089	83.058	56.969	0.0	-0.364	-0.364
-10	4	4	28.291	29.440	-1.149	0.0	-1.110	-1.110

Table 2 (cont)  
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HCLS H REFINEMENT - ALL OTHERS FIXED ANISOTROPIC- CYCLE 32(9-22-77)		STRUCTURE FACTORS						
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
12	4	9	47.296	46.939	46.939	0.0	0.357	0.116
14	4	9	57.505	58.588	58.588	0.0	-1.082	-0.352
14	4	9	41.824	41.824	41.824	0.0	4.116	1.338
16	4	9	16.620	16.527	16.527	0.0	3.096	1.007
16	4	9	47.296	46.719	46.719	0.0	-0.577	-0.142
18	4	9	49.787	47.523	47.523	0.0	2.264	0.773
18	4	9	96.007	97.219	97.219	0.0	1.224	0.441
18	4	9	115.101	114.528	114.528	0.0	0.573	0.184
19	4	9	199.301	200.658	200.658	0.0	-1.357	-0.441
19	4	9	40.008	39.862	39.862	0.0	0.146	0.044
21	4	9	4.859	8.346	8.346	0.0	3.487	1.134
21	4	9	24.171	21.574	21.574	0.0	2.597	0.857
27	4	9	72.646	71.813	71.813	0.0	0.834	0.278
27	4	9	95.374	98.984	98.984	0.0	-3.610	-1.173
27	4	9	18.974	6.052	6.052	0.0	12.922	4.202
29	4	9	151.998	149.991	149.991	0.0	2.007	0.655
31	4	9	86.918	86.918	86.918	0.0	0.000	0.000
31	4	9	15.591	14.339	14.339	0.0	1.252	0.407
31	4	9	26.108	18.048	18.048	0.0	8.060	2.621
33	4	9	119.547	119.868	119.868	0.0	-0.321	-0.104
33	4	9	93.481	88.841	88.841	0.0	4.640	1.495
33	4	9	16.514	20.101	20.101	0.0	-3.587	-1.166
33	4	9	31.920	34.949	34.949	0.0	-3.029	-0.985
33	4	9	70.852	66.207	66.207	0.0	4.645	1.510
33	4	9	138.659	140.277	140.277	0.0	-1.618	-0.526
33	4	9	39.208	31.551	31.551	0.0	7.657	2.490
33	4	9	87.888	88.750	88.750	0.0	-0.862	-0.280
33	4	9	57.967	55.887	55.887	0.0	2.080	0.672
33	4	9	3.567	15.166	15.166	0.0	-11.599	-3.512
33	4	9	52.432	44.708	44.708	0.0	7.724	2.384
33	4	9	25.309	17.056	17.056	0.0	8.257	2.584
33	4	9	28.476	32.472	32.472	0.0	-4.006	-1.199
33	4	9	100.804	5.031	5.031	0.0	95.773	28.746
33	4	9	101.300	101.300	101.300	0.0	0.000	0.000
33	4	9	46.854	46.854	46.854	0.0	0.000	0.000
33	4	9	0.790	0.790	0.790	0.0	0.000	0.000
33	4	9	88.466	88.466	88.466	0.0	0.000	0.000
33	4	9	120.603	120.603	120.603	0.0	0.000	0.000
33	4	9	92.003	92.003	92.003	0.0	0.000	0.000
33	4	9	104.444	104.444	104.444	0.0	0.000	0.000
33	4	9	0.736	0.736	0.736	0.0	0.000	0.000
33	4	9	52.514	52.514	52.514	0.0	0.000	0.000
33	4	9	135.010	135.010	135.010	0.0	0.000	0.000
33	4	9	39.772	39.772	39.772	0.0	0.000	0.000
33	4	9	31.246	31.246	31.246	0.0	0.000	0.000
33	4	9	89.614	89.614	89.614	0.0	0.000	0.000
33	4	9	99.303	99.303	99.303	0.0	0.000	0.000
33	4	9	62.622	62.622	62.622	0.0	0.000	0.000
33	4	9	24.220	24.220	24.220	0.0	0.000	0.000
33	4	9	87.427	87.427	87.427	0.0	0.000	0.000
33	4	9	97.361	97.361	97.361	0.0	0.000	0.000
33	4	9	26.477	23.252	23.252	0.0	3.225	1.049

Table 2 (cont)  
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HCLB H REFINEMENT - ALL OTHERS FIXED ANISOTROPIC - CYCLE 32(9-22-77)				STRUCTURE FACTORS				
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
-2	-4	10	45.482	47.782	47.782	0.0	-2.300	-0.748
-4	-4	10	57.171	48.068	48.068	0.0	3.103	1.009
-4	-4	10	74.210	74.210	74.210	0.0	-1.821	-0.592
-6	-4	10	110.773	0.251	1.251	0.0	18.442	5.991
-6	-4	10	110.773	0.251	1.251	0.0	13.477	4.370
-8	-4	10	134.057	5.226	5.226	0.0	-11.425	-0.467
-8	-4	10	134.057	5.226	5.226	0.0	-11.048	-0.393
-10	-4	10	157.324	27.227	27.227	0.0	-10.210	-0.368
-12	-4	10	157.324	27.227	27.227	0.0	-1.426	-0.064
-12	-4	10	157.324	27.227	27.227	0.0	0.323	0.098
-12	-4	10	157.324	27.227	27.227	0.0	0.552	0.164
-12	-4	10	157.324	27.227	27.227	0.0	2.729	0.823
-12	-4	10	157.324	27.227	27.227	0.0	1.037	0.307
-12	-4	10	157.324	27.227	27.227	0.0	0.203	0.064
-12	-4	10	157.324	27.227	27.227	0.0	0.442	0.131
-12	-4	10	157.324	27.227	27.227	0.0	0.611	0.181
-12	-4	10	157.324	27.227	27.227	0.0	0.653	0.193
-12	-4	10	157.324	27.227	27.227	0.0	0.463	0.137
-12	-4	10	157.324	27.227	27.227	0.0	1.141	0.331
-12	-4	10	157.324	27.227	27.227	0.0	0.211	0.064
-12	-4	10	157.324	27.227	27.227	0.0	0.539	0.158
-12	-4	10	157.324	27.227	27.227	0.0	1.786	0.511
-12	-4	10	157.324	27.227	27.227	0.0	0.710	0.211
-12	-4	10	157.324	27.227	27.227	0.0	0.585	0.171
-12	-4	10	157.324	27.227	27.227	0.0	0.756	0.211
-12	-4	10	157.324	27.227	27.227	0.0	0.002	0.002
-12	-4	10	157.324	27.227	27.227	0.0	1.226	0.344
-12	-4	10	157.324	27.227	27.227	0.0	0.653	0.193
-12	-4	10	157.324	27.227	27.227	0.0	0.239	0.071
-12	-4	10	157.324	27.227	27.227	0.0	0.715	0.211
-12	-4	10	157.324	27.227	27.227	0.0	1.456	0.411
-12	-4	10	157.324	27.227	27.227	0.0	0.920	0.264
-12	-4	10	157.324	27.227	27.227	0.0	0.455	0.137
-12	-4	10	157.324	27.227	27.227	0.0	0.531	0.158
-12	-4	10	157.324	27.227	27.227	0.0	1.700	0.483
-12	-4	10	157.324	27.227	27.227	0.0	0.593	0.171
-12	-4	10	157.324	27.227	27.227	0.0	0.370	0.109
-12	-4	10	157.324	27.227	27.227	0.0	1.047	0.293
-12	-4	10	157.324	27.227	27.227	0.0	1.792	0.511
-12	-4	10	157.324	27.227	27.227	0.0	0.927	0.264
-12	-4	10	157.324	27.227	27.227	0.0	2.160	0.611
-12	-4	10	157.324	27.227	27.227	0.0	1.537	0.431
-12	-4	10	157.324	27.227	27.227	0.0	1.845	0.511
-12	-4	10	157.324	27.227	27.227	0.0	4.457	1.264
-12	-4	10	157.324	27.227	27.227	0.0	1.450	0.411



Table 2 (cont)  
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HCLB F REFINEMENT - ALL OTHERS FIXED ANISOTROPIC- CYCLE 32(9-22-77)									
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
5	5	1	39.306	36.001	36.001	0.0	-6.695	-2.177	
5	5	1	108.061	108.372	108.372	0.0	0.101	-0.101	*
5	5	1	14.645	14.672	14.672	0.0	0.027	0.027	**
5	5	1	23.695	23.613	23.613	0.0	-8.082	-8.082	
5	5	1	25.954	25.959	25.959	0.0	0.005	0.005	
5	5	1	45.400	45.871	45.871	0.0	0.471	0.471	
5	5	1	53.225	54.744	54.744	0.0	1.519	1.519	*
5	5	1	8.426	9.938	9.938	0.0	1.512	-0.492	**
5	5	1	59.653	59.933	59.933	0.0	0.280	0.280	
5	5	1	22.616	20.192	20.192	0.0	-2.424	1.764	
5	5	1	32.720	35.599	35.599	0.0	2.879	-0.936	
5	5	1	44.559	52.960	52.960	0.0	8.401	-2.732	*
5	5	1	15.530	13.347	13.347	0.0	-2.183	0.710	**
5	5	1	100.250	100.058	100.058	0.0	-0.192	0.063	
5	5	1	145.824	145.629	145.629	0.0	-0.195	0.063	
5	5	1	73.958	71.874	71.874	0.0	-2.084	0.677	
5	5	1	100.312	99.721	99.721	0.0	-0.591	0.192	
5	5	1	97.452	99.826	99.826	0.0	2.374	-0.764	
5	5	1	26.477	32.377	32.377	0.0	5.900	-0.772	
5	5	1	61.472	66.359	66.359	0.0	4.887	-1.919	
5	5	1	159.939	162.700	162.700	0.0	2.761	-1.589	
5	5	1	35.949	37.983	37.983	0.0	2.034	-0.898	
5	5	1	27.259	57.424	57.424	0.0	30.165	-0.661	
5	5	1	44.456	40.741	40.741	0.0	-3.715	0.051	
5	5	1	37.794	40.217	40.217	0.0	2.423	1.202	*
5	5	1	16.729	21.785	21.785	0.0	5.056	-0.788	**
5	5	1	59.837	77.237	77.237	0.0	17.400	-1.405	
5	5	1	130.602	123.086	123.086	0.0	-7.516	2.444	
5	5	1	29.737	38.011	38.011	0.0	8.274	-2.691	
5	5	1	61.134	60.735	60.735	0.0	-0.399	0.130	
5	5	1	15.830	13.026	13.026	0.0	-2.804	-0.189	
5	5	1	18.605	10.091	10.091	0.0	-8.514	0.769	
5	5	1	106.862	106.585	106.585	0.0	-0.277	0.270	*
5	5	1	69.437	74.186	74.186	0.0	4.748	-1.540	**
5	5	1	12.977	12.743	12.743	0.0	-0.234	0.076	*
5	5	1	20.942	13.869	13.869	0.0	-7.073	3.070	**
5	5	1	8.974	10.705	10.705	0.0	1.731	-0.727	*
5	5	1	45.974	43.708	43.708	0.0	-2.265	0.265	**
5	5	1	88.020	89.504	89.504	0.0	1.484	-0.285	
5	5	1	39.454	37.945	37.945	0.0	-1.509	0.491	
5	5	1	76.326	77.608	77.608	0.0	1.282	-0.282	
5	5	1	87.304	84.767	84.767	0.0	-2.537	0.537	*
5	5	1	32.396	38.332	38.332	0.0	5.936	-1.605	
5	5	1	32.443	27.857	27.857	0.0	-4.586	1.491	
5	5	1	87.058	88.105	88.105	0.0	1.048	-0.048	
5	5	1	187.093	187.871	187.871	0.0	0.778	-0.251	
5	5	1	66.761	69.154	69.154	0.0	2.393	-0.128	
5	5	1	100.329	99.984	99.984	0.0	-0.345	0.112	*
5	5	1	18.153	105.928	105.928	0.0	2.225	0.724	**
5	5	1	16.468	17.468	17.468	0.0	1.000	-0.985	
5	5	1	42.929	153.801	153.801	0.0	110.872	0.454	*
5	5	1	59.441	59.441	59.441	0.0	0.000	1.134	



Table 2 (cont)  
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H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
1	5	4	19.404	11.414	11.414	0.0	7.990	2.598
1	5	4	49.329	50.358	-28.379	0.0	-1.029	-0.534
1	5	4	40.654	42.237	-42.834	0.0	-2.417	-1.762
1	5	4	49.414	46.801	-43.801	0.0	-0.051	-0.051
1	5	4	77.125	73.801	-73.801	0.0	3.324	2.308
1	5	4	83.757	76.800	-76.800	0.0	3.958	1.137
1	5	4	35.303	38.800	-38.800	0.0	-0.375	-0.375
1	5	4	124.300	124.567	124.567	0.0	-1.153	-0.067
1	5	4	8.426	6.388	32.889	0.0	2.038	0.663
1	5	4	39.700	48.431	-48.431	0.0	2.241	0.681
1	5	4	50.525	22.319	-22.319	0.0	1.362	0.681
1	5	4	26.508	28.890	-28.890	0.0	4.189	0.125
1	5	4	29.275	24.830	-24.830	0.0	0.385	0.125
1	5	4	8.610	36.830	-36.830	0.0	-15.220	-5.274
1	5	4	35.525	23.752	-23.752	0.0	-1.311	-0.426
1	5	4	23.525	18.720	-18.720	0.0	0.226	0.496
1	5	4	20.295	17.696	-17.696	0.0	1.861	0.496
1	5	4	21.527	14.177	-14.177	0.0	7.157	2.327
1	5	4	14.064	16.804	-16.804	0.0	-0.720	-0.884
1	5	4	20.644	12.109	-12.109	0.0	2.472	0.772
1	5	4	27.154	26.428	-26.428	0.0	0.726	0.246
1	5	4	45.411	45.471	45.471	0.0	-0.060	-0.060
1	5	4	103.500	99.859	-99.859	0.0	3.641	0.007
1	5	4	24.000	21.955	-21.955	0.0	2.045	1.187
1	5	4	17.000	18.992	-18.992	0.0	-1.992	-0.687
1	5	4	91.002	79.857	-79.857	0.0	1.145	0.616
1	5	4	33.222	24.703	-24.703	0.0	8.509	0.401
1	5	4	25.801	25.600	-25.600	0.0	0.201	2.797
1	5	4	93.811	60.334	-60.334	0.0	3.477	0.036
1	5	4	36.041	35.816	-35.816	0.0	0.225	0.150
1	5	4	60.500	60.802	60.802	0.0	-0.302	-0.063
1	5	4	79.493	77.073	-77.073	0.0	2.420	0.782
1	5	4	24.309	25.231	-25.231	0.0	-0.922	-0.182
1	5	4	105.048	105.962	105.962	0.0	-0.914	-0.292
1	5	4	19.004	8.236	-8.236	0.0	10.769	0.502
1	5	4	21.188	22.738	-22.738	0.0	-1.551	-0.502
1	5	4	15.020	6.966	6.966	0.0	8.064	0.515
1	5	4	27.584	24.827	-24.827	0.0	2.757	1.093
1	5	4	70.575	64.852	-64.852	0.0	-1.510	-0.481
1	5	4	27.061	42.416	-42.416	0.0	2.001	0.651
1	5	4	18.005	17.501	-17.501	0.0	0.504	0.220
1	5	4	29.508	26.507	-26.507	0.0	0.001	0.000
1	5	4	47.450	40.591	-40.591	0.0	6.859	2.230
1	5	4	31.322	9.844	-9.844	0.0	-2.512	-0.817
1	5	4	47.444	5.225	-5.225	0.0	-0.310	-0.310
1	5	4	17.702	196.023	-196.023	0.0	-1.279	-0.416
1	5	4	32.714	74.333	-74.333	0.0	0.929	0.302
1	5	4	37.911	37.911	37.911	0.0	0.805	0.265
1	5	4	38.451	97.436	-97.436	0.0	0.815	0.265

Table 2 (cont)  
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HCLB H REFINEMENT - ALL OTHERS FIXED ANISOTROPIC- CYCLE 32(9-22-77)

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
0	5	8	183.956	175.850	175.850	0.000	8.106	2.636	
-10	5	8	132.592	27.070	-27.070	0.000	-13.477	-4.383	**
-15	5	8	49.848	100.635	-100.635	0.000	1.525	0.525	**
0	5	8	59.222	46.028	46.028	0.000	-6.803	1.242	
0	5	8	40.158	74.800	-74.800	0.000	4.358	-1.417	
0	5	8	35.518	41.800	-41.800	0.000	1.500	0.511	**
0	5	8	29.737	20.262	-20.262	0.000	10.012	-2.179	
0	5	8	29.099	16.725	-16.725	0.000	3.374	3.256	
0	5	8	29.854	120.131	-120.131	0.000	-0.691	1.097	
0	5	8	44.213	45.004	-45.004	0.000	11.598	-0.225	
0	5	8	22.449	28.713	-28.713	0.000	3.611	0.157	
0	5	8	40.039	10.751	-10.751	0.000	6.352	2.804	
0	5	8	139.198	138.908	138.908	0.000	-0.231	2.066	
0	5	8	50.617	54.145	-54.145	0.000	3.528	1.147	
0	5	8	43.421	41.225	-41.225	0.000	2.136	0.714	
0	5	8	76.141	62.744	-62.744	0.000	3.179	-0.774	
0	5	8	41.576	72.952	-72.952	0.000	3.893	1.034	
0	5	8	38.954	45.229	-45.229	0.000	1.647	1.198	
0	5	8	20.019	83.901	-83.901	0.000	1.251	3.554	**
0	5	8	14.322	19.708	-19.708	0.000	5.710	-1.798	**
0	5	8	34.063	30.023	-30.023	0.000	4.475	1.766	**
0	5	8	128.255	128.255	128.255	0.000	4.702	1.402	
0	5	8	31.820	24.005	-24.005	0.000	7.314	1.302	
0	5	8	46.927	52.028	-52.028	0.000	5.716	2.574	
0	5	8	22.110	20.007	-20.007	0.000	-1.703	1.737	
0	5	8	13.930	18.516	-18.516	0.000	-14.054	0.684	**
0	5	8	18.651	27.984	-27.984	0.000	0.305	4.570	**
0	5	8	54.701	57.810	-57.810	0.000	0.892	2.241	**
0	5	8	25.771	23.779	-23.779	0.000	-3.008	0.002	*
0	5	8	70.505	10.952	-10.952	0.000	4.442	1.121	**
0	5	8	9.025	26.064	-26.064	0.000	0.988	1.344	*
0	5	8	58.231	80.081	-80.081	0.000	-3.233	0.321	**
0	5	8	16.288	29.361	-29.361	0.000	-1.062	4.358	*
0	5	8	107.893	107.893	107.893	0.000	0.300	0.300	**
0	5	8	19.042	31.070	-31.070	0.000	-1.096	1.300	*
0	5	8	14.024	15.997	-15.997	0.000	-10.512	0.156	**
0	5	8	14.024	16.914	-16.914	0.000	-3.373	1.426	**
0	5	8	45.074	49.184	-49.184	0.000	-3.210	0.718	**
0	5	8	33.033	74.586	-74.586	0.000	1.654	3.444	**
0	5	8	11.258	93.868	-93.868	0.000	-5.580	1.851	**
0	5	8	17.771	18.229	-18.229	0.000	1.974	1.044	**
0	5	8	101.050	176.618	-176.618	0.000	1.153	0.325	*
0	5	8	24.920	103.132	-103.132	0.000	-5.082	-0.572	**
0	5	8	71.024	20.512	-20.512	0.000	-12.699	-1.203	**
0	5	8	8.180	20.653	-20.653	0.000	-12.473	-4.056	**

Table 2 (cont.)  
PAGE 24

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
-14	0	0	62.672	60.532	-60.532	0.00	2.140	0.696	
-14	0	0	37.028	40.441	40.441	0.00	-4.413	-0.801	
13	0	0	85.080	89.892	89.892	0.00	-4.812	-1.582	
5	0	0	12.254	14.870	14.870	0.00	-2.616	-0.907	**
5	0	0	59.276	77.203	77.203	0.00	-17.927	-2.523	**
5	0	0	26.754	12.122	12.122	0.00	14.632	4.683	**
7	0	0	11.440	17.591	17.591	0.00	-6.151	-1.255	**
0	0	0	70.860	82.371	82.371	0.00	-11.511	-0.881	
0	0	0	23.700	153.381	153.381	0.00	-129.681	-5.960	
11	0	0	180.001	180.974	180.974	0.00	-0.973	-1.121	
11	0	0	44.774	42.658	42.658	0.00	2.116	0.603	**
11	0	0	15.944	72.574	72.574	0.00	-56.630	-3.168	**
11	0	0	71.251	37.700	37.700	0.00	33.551	1.700	
15	0	0	24.724	25.876	25.876	0.00	-1.152	-0.362	**
15	0	0	15.038	11.876	11.876	0.00	3.162	1.113	**
0	0	0	97.636	98.058	98.058	0.00	-0.422	-0.140	
2	0	0	38.962	40.520	40.520	0.00	-1.558	-0.539	
2	0	0	18.380	23.020	23.020	0.00	-4.640	-1.517	**
4	0	0	41.452	44.020	44.020	0.00	-2.568	-0.836	**
4	0	0	109.322	104.067	104.067	0.00	5.255	1.406	
4	0	0	85.151	83.060	83.060	0.00	2.091	0.697	**
6	0	0	17.733	19.370	19.370	0.00	-1.637	-0.529	**
8	0	0	114.622	114.622	114.622	0.00	0.000	0.000	
10	0	0	157.659	160.611	160.611	0.00	-2.952	-0.960	
10	0	0	115.780	113.174	113.174	0.00	2.606	0.847	
12	0	0	26.231	24.710	24.710	0.00	1.521	0.492	
12	0	0	47.850	46.919	46.919	0.00	0.931	0.303	
14	0	0	24.847	29.785	29.785	0.00	-4.938	-1.498	
14	0	0	50.555	50.710	50.710	0.00	-0.155	-0.046	
1	0	0	41.299	40.312	40.312	0.00	0.987	0.311	
3	0	0	53.865	55.961	55.961	0.00	-2.096	-0.688	
3	0	0	75.833	71.114	71.114	0.00	4.719	1.549	
3	0	0	80.588	84.610	84.610	0.00	-4.022	-1.324	**
5	0	0	19.158	12.312	12.312	0.00	6.846	2.200	**
7	0	0	21.598	36.112	36.112	0.00	-14.514	-4.723	**
7	0	0	46.988	43.675	43.675	0.00	3.313	1.077	**
9	0	0	92.310	90.147	90.147	0.00	2.163	0.835	**
11	0	0	16.310	28.248	28.248	0.00	-11.938	-3.866	**
11	0	0	35.344	40.558	40.558	0.00	-5.214	-1.699	**
11	0	0	16.520	30.749	30.749	0.00	-14.229	-4.619	**
13	0	0	12.218	12.218	12.218	0.00	0.000	0.000	**
13	0	0	64.842	64.842	64.842	0.00	0.000	0.000	**
1	0	0	9.191	3.842	3.842	0.00	5.349	1.531	**
2	0	0	15.282	4.331	4.331	0.00	10.951	3.642	**
2	0	0	95.084	97.890	97.890	0.00	-2.806	-0.913	**
4	0	0	56.577	59.825	59.825	0.00	-3.248	-1.056	**
4	0	0	70.483	68.600	68.600	0.00	1.883	0.612	**
4	0	0	56.706	63.170	63.170	0.00	-6.464	-2.102	**
4	0	0	1.577	1.102	1.102	0.00	0.475	0.162	**
8	0	0	83.675	83.740	83.740	0.00	-0.065	-0.021	**

Table 2 (cont)  
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HCLB H REFINEMENT - ALL OTHERS FIXED ANISOTROPIC - CYCLE 32(8-22-77)									
M	K	L	F(JSS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
10	0	4	115.642	114.943	114.943	0.0	0.059	0.032	
10	0	4	95.091	95.459	-65.979	0.0	-0.368	-0.116	
11	0	4	25.741	45.970	-65.979	0.0	14.002	4.553	
11	0	4	10.741	45.174	-43.134	0.0	-3.634	-1.224	
11	0	5	10.005	10.210	110.297	0.0	-4.073	-1.324	
11	0	5	3.471	11.297	110.297	0.0	8.696	2.828	
11	0	5	3.087	52.742	-42.099	0.0	-5.163	-1.679	
11	0	5	10.772	87.697	-87.697	0.0	1.390	0.452	
11	0	5	5.764	100.599	-100.599	0.0	1.773	0.577	
11	0	5	5.414	57.135	-27.405	0.0	8.359	2.718	
11	0	5	5.175	44.310	-13.310	0.0	2.279	0.741	**
11	0	5	5.037	67.312	-95.514	0.0	0.894	0.291	
11	0	5	5.020	54.894	-55.312	0.0	2.856	0.932	
11	0	5	5.020	44.363	46.994	0.0	3.117	0.886	
11	0	5	5.020	80.441	96.368	0.0	1.888	0.614	
11	0	5	5.020	78.441	78.449	0.0	2.846	0.925	
11	0	5	5.020	58.679	-58.671	0.0	-3.223	-1.048	
11	0	5	5.020	10.971	10.971	0.0	7.971	2.365	**
11	0	5	5.020	49.102	49.102	0.0	-3.936	-1.117	
11	0	5	5.020	30.770	30.770	0.0	-3.770	-1.226	
11	0	5	5.020	44.747	-44.747	0.0	0.119	0.071	
11	0	5	7.755	72.844	-72.844	0.0	4.111	1.532	
11	0	5	8.6105	80.999	-80.999	0.0	-5.106	-1.600	*
11	0	5	15.816	11.411	-11.411	0.0	-3.134	-1.221	**
11	0	5	19.877	77.445	-77.445	0.0	3.250	1.175	
11	0	5	17.805	20.814	-20.814	0.0	17.971	5.116	**
11	0	5	19.691	93.789	93.789	0.0	7.971	2.562	
11	0	5	43.913	48.605	48.605	0.0	0.491	0.101	
11	0	5	11.553	10.946	-10.946	0.0	-0.491	-0.200	**
11	0	5	44.159	45.873	-45.873	0.0	-1.074	-0.357	
11	0	5	9.4715	99.471	99.471	0.0	-1.754	-0.546	
11	0	5	42.960	39.755	39.755	0.0	3.704	1.082	
11	0	5	45.420	9.114	-9.114	0.0	17.235	5.219	
11	0	5	19.174	40.725	40.725	0.0	14.695	4.219	
11	0	5	10.511	9.390	9.390	0.0	8.784	2.527	**
11	0	5	8.703	102.949	-102.949	0.0	-8.438	-2.498	**
11	0	5	19.112	1.158	-1.158	0.0	-7.545	-2.272	**
11	0	5	45.612	25.285	-25.285	0.0	-7.173	-2.272	**
11	0	5	54.031	46.949	-46.949	0.0	-11.476	-3.627	
11	0	5	25.821	55.795	-55.795	0.0	-1.765	-0.542	
11	0	5	17.971	27.190	-27.190	0.0	-1.358	-0.412	
11	0	5	17.325	89.700	-89.700	0.0	4.277	1.391	
11	0	5	97.175	173.338	173.338	0.0	-2.072	-0.671	
11	0	5	97.008	96.644	96.644	0.0	0.531	0.173	
11	0	5	36.010	70.879	70.879	0.0	-3.871	-1.259	
11	0	5	27.069	22.910	-22.910	0.0	13.100	4.260	
11	0	5	21.649	62.774	-62.774	0.0	-4.295	-1.397	
11	0	5	32.070	32.070	32.070	0.0	-10.421	-3.289	**

Table 2 (cont)  
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MCLS H REFINEMENT - ALL OTHERS FIXED ANISOTROPIC - CYCLE 32(9-22-77)				STRUCTURE FACTORS				
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	0	0	34.706	53.845	53.845	0.0	2.874	0.930
1	0	0	52.124	49.450	49.450	0.0	0.820	0.820
1	0	0	31.058	31.624	31.624	0.0	0.466	0.466
1	0	0	33.432	53.256	53.256	0.0	-0.268	-0.268
1	0	0	35.446	27.994	27.994	0.0	-1.552	-1.552
1	0	0	35.109	59.189	59.189	0.0	-5.053	-5.053
1	0	0	31.233	37.789	37.789	0.0	-0.997	-0.997
1	0	0	31.257	52.255	52.255	0.0	-0.324	-0.324
1	0	0	11.955 *	10.485	10.485	0.0	0.380	0.380
1	0	0	37.715	92.150	92.150	0.0	1.170	1.170
1	0	0	37.070	73.129	73.129	0.0	2.565	2.565
1	0	0	40.951	42.550	42.550	0.0	-0.645	-0.645
1	0	0	54.951	40.344	40.344	0.0	0.187	0.187
1	0	0	11.440 *	47.101	47.101	0.0	0.061	0.061
1	0	0	38.553	12.653	12.653	0.0	7.852	7.852
1	0	0	26.170	42.725	42.725	0.0	-0.394	-0.394
1	0	0	27.451	16.607	16.607	0.0	-0.704	-0.704
1	0	0	25.216	75.100	75.100	0.0	3.100	3.100
1	0	0	57.249	18.700	18.700	0.0	-0.862	-0.862
1	0	0	19.271	72.528	72.528	0.0	6.461	6.461
1	0	0	43.667	118.008	118.008	0.0	-4.812	-4.812
1	0	0	36.459	15.925	15.925	0.0	-0.727	-0.727
1	0	0	37.352	56.244	56.244	0.0	7.742	7.742
1	0	0	26.262	20.550	20.550	0.0	2.218	2.218
1	0	0	45.758	16.888	16.888	0.0	-0.634	-0.634
1	0	0	34.448	45.415	45.415	0.0	3.327	3.327
1	0	0	132.649	16.665	16.665	0.0	9.374	9.374
1	0	0	179.493	99.897	99.897	0.0	0.586	0.586
1	0	0	28.138	77.624	77.624	0.0	7.782	7.782
1	0	0	41.638	30.987	30.987	0.0	1.869	1.869
1	0	0	23.217	36.831	36.831	0.0	4.627	4.627
1	0	0	23.925	21.770	21.770	0.0	1.447	1.447
1	0	0	54.997	82.370	82.370	0.0	2.521	2.521
1	0	0	100.589	105.040	105.040	0.0	-0.452	-0.452
1	0	0	56.885	66.863	66.863	0.0	0.448	0.448
1	0	0	118.662	24.885	24.885	0.0	0.007	0.007
1	0	0	49.479	118.774	118.774	0.0	-0.507	-0.507
1	0	0	99.622	53.137	53.137	0.0	-0.558	-0.558
1	0	0	99.891	69.082	69.082	0.0	0.540	0.540
1	0	0	12.943	33.800	33.800	0.0	-0.376	-0.376
1	0	0	13.900 *	76.356	76.356	0.0	-3.457	-3.457
1	0	0	21.342	22.551	22.551	0.0	2.681	2.681
1	0	0	78.048	8.589	8.589	0.0	4.347	4.347
1	0	0	48.056	76.343	76.343	0.0	0.254	0.254
1	0	0	76.261	41.893	41.893	0.0	-0.570	-0.570
1	0	0	27.184	-76.361	-76.361	0.0	0.343	0.343
1	0	0	106.403	1.616	1.616	0.0	-8.115	-8.115
1	0	0	30.592	-106.403	-106.403	0.0	1.167	1.167
1	0	0	31.248	36.337	36.337	0.0	4.255	4.255
1	0	0		24.223	24.223	0.0	7.021	7.021

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\*

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
1	7	4	61.534	57.569	-57.569	0.0	3.965	1.289	
1	7	4	101.987	101.581	-101.581	0.0	1.407	0.457	
1	7	4	120.320	120.429	120.429	0.0	-0.109	0.685	
1	7	4	120.279	120.445	120.445	0.0	-0.166	0.044	
1	7	4	133.282	133.524	133.524	0.0	-0.242	0.572	
1	7	4	151.661	150.710	-9.951	0.0	0.951	0.798	
1	7	5	80.231	82.565	2.334	0.0	-2.334	0.758	
1	7	5	87.725	89.921	2.196	0.0	-2.196	1.655	
1	7	5	87.738	90.920	2.182	0.0	-2.182	0.341	
1	7	5	98.121	96.980	-1.141	0.0	1.141	1.573	
1	7	5	93.287	93.390	0.103	0.0	-0.103	0.596	
1	7	5	93.765	92.139	-1.626	0.0	1.626	1.265	
1	7	5	93.255	91.599	-1.656	0.0	1.656	0.530	
1	7	6	43.742	43.742	0.0	0.0	0.0	0.024	
1	7	6	31.244	34.305	3.061	0.0	-3.061	0.096	
1	7	6	37.886	41.253	3.367	0.0	-3.367	0.095	
1	7	6	19.340	24.975	5.635	0.0	-5.635	2.002	*
1	7	6	145.886	100.600	-45.286	0.0	45.286	1.216	*
1	7	6	142.602	145.079	2.477	0.0	-2.477	0.276	
1	7	6	130.049	122.016	-7.033	0.0	7.033	3.422	
1	7	7	43.698	32.812	-10.886	0.0	10.886	0.955	
1	7	7	55.375	61.439	5.064	0.0	-5.064	1.281	
1	7	7	33.325	41.671	8.346	0.0	-8.346	1.374	*
1	7	7	39.270	43.436	4.166	0.0	-4.166	0.302	*
1	7	7	22.387	26.426	4.039	0.0	-4.039	0.512	*
1	7	7	31.059	30.129	-0.930	0.0	0.930	2.844	*
1	7	8	18.625	27.380	8.755	0.0	-8.755	0.212	*
1	7	8	71.528	69.931	-1.597	0.0	1.597	1.432	*
1	7	8	44.857	40.444	-4.413	0.0	4.413	0.585	*
1	7	8	48.618	46.880	-1.738	0.0	1.738	3.190	*
1	7	8	70.144	79.955	9.811	0.0	-9.811	2.139	*
1	7	8	145.898	20.318	-125.580	0.0	125.580	0.203	*
1	7	8	133.898	117.311	-16.587	0.0	16.587	0.580	*
1	7	8	56.214	63.162	6.948	0.0	-6.948	1.853	*
1	7	8	19.227	17.677	-1.550	0.0	1.550	0.222	*
1	7	8	140.227	142.012	1.785	0.0	-1.785	0.522	*
1	7	8	19.588	13.861	-5.727	0.0	5.727	1.853	*
1	7	8	109.476	107.923	-1.553	0.0	1.553	0.522	*
1	7	8	53.334	52.857	-0.477	0.0	0.477	0.222	*
1	7	8	35.344	55.881	20.537	0.0	-20.537	0.822	*
1	7	8	129.235	32.019	-97.216	0.0	97.216	4.786	*
1	7	8	129.235	145.893	26.658	0.0	-26.658	0.822	*
1	7	8	129.235	105.934	-23.301	0.0	23.301	0.822	*
1	7	8	129.235	161.954	32.719	0.0	-32.719	0.822	*
1	7	8	129.235	13.366	-115.869	0.0	115.869	2.443	*
1	7	8	129.235	114.050	-114.050	0.0	0.0	0.822	*
1	7	8	129.235	126.181	-7.054	0.0	7.054	2.344	*
1	7	8	76.725	74.039	-2.686	0.0	2.686	0.822	*



Table 2 (cont)  
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HCLB H REFINEMENT - ALL OTHERS FIXED ANISOTROPIC- CYCLE 32(9-22-77)									
H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
1	-8	3	19.374 *	12.970	-12.970	0.0	6.404	2.082	* **
-1	-8	3	32.197	30.263	-30.263	0.0	1.934	0.629	
3	-8	3	32.474	29.453	-29.453	0.0	3.021	0.982	
5	-8	3	35.089	27.613	-27.613	0.0	7.475	2.431	
-5	-8	3	50.433	53.773	53.773	0.0	-3.339	-1.086	
0	-8	4	37.056	19.328	19.328	0.0	17.728	5.765	
2	-8	4	32.566	28.830	28.830	0.0	3.730	1.213	
-2	-8	4	38.593	41.851	41.851	0.0	-3.258	-1.059	* **
-4	-8	4	8.926 *	2.181	2.181	0.0	6.745	2.161	
-1	-8	5	110.368	109.417	-109.417	0.0	0.951	0.309	



Table 3. Thermal Ellipsoids for Calcium, Chlorine, and Oxygen Atoms of Hydrochlorborite

Atom	Ellipsoid axes	RMS amplitude, Å	Angles (°) to crystal axes		
			a	b	c
Ca(1)	1	0.100(5)	113(5)	128(14)	44(13)
	2	.114(5)	85(8)	140(14)	130(14)
	3	.143(4)	24(5)	101(6)	76(5)
Ca(2)	1	0.099(5)	112(6)	107(9)	23(6)
	2	.122(4)	68(13)	157(11)	100(10)
	3	.137(4)	32(10)	74(12)	69(5)
Cl	1	0.141(5)	100(9)	96(16)	7(11)
	2	.153(5)	61(7)	151(8)	95(15)
	3	.190(4)	31(5)	62(5)	85(4)
O(1)	1	0.08(2)	89(11)	85(23)	9(12)
	2	.11(1)	108(17)	18(18)	93(24)
	3	.15(1)	162(17)	107(17)	81(9)
O(2)	1	0.02(7)	77(14)	94(14)	20(17)
	2	.09(2)	45(11)	133(10)	107(19)
	3	.15(1)	132(9)	137(9)	79(7)
O(3)	1	0.09(2)	31(18)	98(24)	67(25)
	2	.12(2)	74(30)	134(9)	133(19)
	3	.20(1)	116(5)	134(6)	52(6)
O(4)	1	0.08(2)	107(9)	48(6)	44(6)
	2	.15(1)	163(9)	102(17)	95(17)
	3	.17(1)	90(21)	136(9)	46(7)
OH(1)	1	0.03(5)	97(7)	55(10)	35(10)
	2	.12(1)	70(11)	38(11)	123(11)
	3	.17(1)	21(11)	103(10)	80(8)
OH(2)	1	0.09(2)	120(10)	92(12)	23(10)
	2	.14(1)	113(44)	152(52)	102(21)
	3	.15(1)	40(33)	118(52)	70(15)
OH(3)	1	0.06(2)	90(6)	84(9)	9(7)
	2	.14(1)	100(19)	12(17)	95(10)
	3	.17(1)	170(19)	100(19)	82(6)
OH(4)	1	0.11(2)	117(13)	91(17)	21(14)
	2	.14(1)	121(18)	144(18)	103(20)
	3	.17(1)	43(15)	126(18)	74(10)

Table 3 (continued)

Atom	Ellipsoid axes	RMS amplitude, Å	Angles (°) to crystal axes		
			a	b	c
OH(5)	1	0.09(2)	121(10)	121(6)	43(8)
	2	.15(1)	143(12)	89(14)	120(12)
	3	.19(1)	107(14)	31(6)	63(10)
OH(6)	1	0.12(2)	99(24)	148(12)	58(12)
	2	.15(1)	168(24)	187(25)	95(24)
	3	.17(1)	98(23)	58(12)	32(12)
OH(7)	1	0.09(2)	103(6)	115(11)	26(11)
	2	.15(1)	99(15)	151(12)	116(11)
	3	.18(1)	16(10)	104(14)	89(8)
H <sub>2</sub> O(1)	1	0.11(2)	108(5)	99(7)	15(4)
	2	.19(1)	121(9)	31(9)	88(8)
	3	.24(1)	57(8)	61(9)	76(4)
H <sub>2</sub> O(2)	1	0.13(1)	79(9)	25(9)	69(10)
	2	.19(1)	59(68)	76(26)	152(48)
	3	.19(1)	33(66)	110(20)	71(65)
H <sub>2</sub> O(3)	1	0.12(2)	120(13)	77(8)	27(14)
	2	.16(1)	140(13)	70(12)	117(14)
	3	.20(1)	114(13)	156(13)	87(20)
H <sub>2</sub> O(4)	1	0.14(1)	83(13)	102(31)	18(20)
	2	.16(1)	100(24)	165(29)	100(31)
	3	.18(1)	168(21)	82(24)	75(15)
H <sub>2</sub> O(5)	1	0.13(1)	90(16)	164(12)	74(11)
	2	.16(1)	152(18)	98(17)	111(18)
	3	.19(1)	118(18)	76(10)	26(15)
H <sub>2</sub> O(6)	1	0.11(2)	112(5)	98(15)	18(9)
	2	.16(1)	89(11)	171(14)	99(14)
	3	.21(1)	22(5)	93(10)	75(5)
H <sub>2</sub> O(7)	1	0.12(1)	102(8)	79(8)	12(6)
	2	.18(1)	141(16)	129(16)	87(10)
	3	.21(1)	54(16)	139(16)	78(6)

Number in parentheses is one standard deviation; for 0.100(5), read  $0.100 \pm 0.005$  Å, etc.

End of supplemental material.