

The following material did not appear in the original publication.

Table 2. Hydrochlorite: Brown and Clark

H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
-4	0	0	89.949	91.664	91.664	0.0	-1.716	-0.558
-4	0	0	150.757	148.953	148.953	0.0	-1.804	-0.907
-1	0	0	177.214	177.716	197.716	0.0	-2.431	-0.786
-1	0	0	275.817	259.248	-259.248	0.0	-17.440	-5.671
-1	0	0	351.842	35.414	35.414	0.0	-2.202	-0.208
-1	0	0	49.258	52.486	-52.486	0.0	-2.596	-0.844
-2	0	0	93.235	91.884	42.088	0.0	0.671	0.283
-2	0	0	123.128	24.712	-24.712	0.0	-4.807	-0.201
-3	0	0	113.443	110.704	143.935	0.0	1.918	1.564
-3	0	0	225.983	120.510	-120.510	0.0	2.476	0.891
-3	0	0	170.773	182.051	182.051	0.0	1.012	1.130
-10	0	0	170.170	132.425	-132.425	0.0	-3.746	-3.329
-10	0	0	23.623	151.616	-151.616	0.0	-8.531	-2.774
-10	0	0	147.423	27.816	27.816	0.0	-4.192	-1.363
-11	0	0	17.520	25.560	-25.560	0.0	10.852	3.525
-11	0	0	233.559	226.393	-226.393	0.0	-3.212	-1.045
-11	0	0	27.307	138.433	138.433	0.0	0.938	2.934
-11	0	0	147.817	134.054	1174.254	0.0	-3.237	-1.033
-11	0	0	130.817	66.895	66.895	0.0	1.177	1.438
-18	0	0	38.470	42.897	-42.897	0.0	-4.422	-0.978
-2	0	0	6.827	57.818	-57.818	0.0	3.088	0.978
0	0	0	9.656	8.731	-8.731	0.0	0.925	0.301
0	0	0	142.593	150.593	-150.593	0.0	-7.936	-2.581
0	0	0	67.838	67.409	-67.409	0.0	0.429	0.139
0	0	0	78.109	76.757	-76.757	0.0	1.322	0.440
0	0	0	396.142	402.408	-402.408	0.0	-6.268	-2.038
0	0	0	106.155	106.968	-106.968	0.0	-0.813	-0.264
0	0	0	127.615	32.587	32.587	0.0	-1.025	-1.617
0	0	0	190.045	188.972	188.972	0.0	-1.073	-0.349
0	0	0	54.307	58.261	-58.261	0.0	-3.954	-1.288
0	0	0	98.128	90.507	-90.507	0.0	7.623	2.478
0	0	0	73.158	78.545	-78.545	0.0	-5.387	-1.752
0	0	0	22.541	24.155	-24.155	0.0	-1.614	-0.525
0	0	0	141.234	147.132	-147.132	0.0	-5.898	-1.937
0	0	0	166.858	163.339	163.339	0.0	3.480	1.181
0	0	0	37.809	32.046	-32.046	0.0	5.767	1.809
0	0	0	85.920	89.577	-89.577	0.0	-3.657	-1.189
0	0	0	107.599	105.461	-105.461	0.0	2.138	0.688
0	0	0	85.623	88.566	-88.566	0.0	-2.943	-0.951
0	0	0	65.101	58.768	-58.768	0.0	6.337	2.037
0	0	0	14.822	19.322	-19.322	0.0	-4.500	-1.593
0	0	0	155.522	153.304	153.304	0.0	-2.218	-0.738
0	0	0	204.037	213.211	-213.211	0.0	9.174	3.087
0	0	0	199.943	197.214	197.214	0.0	-2.720	-0.887
0	0	0	145.885	150.003	-150.003	0.0	-4.118	-1.349
0	0	0	47.388	41.393	-41.393	0.0	5.995	1.849
0	0	0	207.081	210.050	-210.050	0.0	-2.969	-0.865

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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	STRUCTURE FACTORS
1	0	0	142.841	141.517	-141.517	0.000	1.324	0.431	
1	0	0	322.131	320.274	-30.274	0.000	1.856	1.255	
1	0	0	229.597	229.152	-29.152	0.000	-3.048	-1.207	*
1	0	0	191.097	191.113	9.113	0.000	0.016	0.000	**
1	0	0	159.509	157.694	-191.884	0.000	0.013	0.000	
1	0	0	180.038	181.640	157.970	0.000	1.602	0.530	
1	0	0	120.177	114.743	-181.899	0.000	-0.431	-1.291	
1	0	0	183.491	177.365	-14.586	0.000	-5.126	-1.798	
1	0	0	119.285	36.825	-36.825	0.000	5.529	0.375	
1	0	0	54.769	37.187	-19.121	0.000	1.154	0.375	
1	0	0	63.741	88.197	58.197	0.000	17.452	5.719	
1	0	0	75.674	56.418	-51.677	0.000	4.044	1.565	
1	0	0	58.666	261.594	251.594	0.000	0.744	0.242	*
1	0	0	335.910	355.924	20.014	0.000	-26.373	-2.758	
1	0	0	112.822	113.621	123.224	0.000	1.045	0.340	
1	0	0	122.459	113.770	-113.770	0.000	-0.829	-0.413	
1	0	0	160.705	160.949	160.949	0.000	0.244	0.078	
1	0	0	218.705	218.201	-218.201	0.000	-0.505	-0.164	
1	0	0	26.631	29.124	29.124	0.000	2.493	0.811	
1	0	0	78.326	77.757	-77.757	0.000	-0.569	-0.192	
1	0	0	75.218	75.317	75.317	0.000	0.099	0.032	
1	0	0	99.759	128.726	95.726	0.000	4.126	1.537	
1	0	0	127.681	128.726	128.726	0.000	1.065	0.346	
1	0	0	152.426	155.209	155.209	0.000	2.789	1.032	
1	0	0	103.018	100.599	-100.599	0.000	-2.150	-0.827	
1	0	0	172.359	171.610	-71.610	0.000	0.748	0.243	
1	0	0	151.267	148.663	-56.663	0.000	2.604	0.847	
1	0	0	39.916	31.892	-31.892	0.000	8.019	2.608	
1	0	0	201.854	199.970	-199.970	0.000	1.884	0.629	
1	0	0	204.560	217.083	217.083	0.000	12.523	4.072	
1	0	0	204.621	204.288	-204.288	0.000	-0.333	-0.121	
1	0	0	106.788	110.699	110.699	0.000	3.911	1.298	
1	0	0	47.480	46.124	-46.124	0.000	-1.356	-0.441	
1	0	0	21.926	22.522	22.522	0.000	0.596	0.197	
1	0	0	56.444	170.632	170.632	0.000	11.077	3.572	
1	0	0	136.783	140.845	140.845	0.000	4.061	1.320	
1	0	0	96.837	96.765	-96.765	0.000	-0.072	-0.023	
1	0	0	62.210	60.197	-60.197	0.000	-2.013	-0.685	*
1	0	0	7.823	23.231	23.231	0.000	15.408	5.004	**
1	0	0	54.523	225.990	225.990	0.000	17.461	5.004	
1	0	0	32.032	53.206	53.206	0.000	21.171	6.655	
1	0	0	97.300	97.555	97.555	0.000	0.255	0.043	
1	0	0	45.657	39.057	-39.057	0.000	-5.604	-1.971	
1	0	0	167.104	170.133	170.133	0.000	3.029	1.054	
1	0	0	35.026	33.710	-33.710	0.000	-1.316	-0.453	
1	0	0	137.060	145.622	145.622	0.000	8.562	2.784	
1	0	0	225.594	225.476	-225.476	0.000	-0.118	-0.038	
1	0	0	40.469	49.295	49.295	0.000	8.825	2.903	*
1	0	0	11.163	1.006	-1.006	0.000	-10.157	-3.503	**

Table 2 (cont.)
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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
6	0	1	102.985	175.192	175.100	0.000	-14.116	-4.590
8	0	2	154.780	174.275	-34.875	0.000	-10.095	-0.031
8	0	3	122.410	115.217	115.217	0.000	10.198	3.316
1	0	2	112.732	115.129	115.129	0.000	-12.193	-0.778
1	0	2	94.733	96.181	-66.147	0.000	-3.875	-1.260
1	0	2	144.648	16.004	-16.004	0.000	-1.340	-0.436
1	0	2	27.402	80.722	-66.722	0.000	-2.575	-0.870
2	0	4	27.830	19.404	-10.404	0.000	-3.092	-0.976
4	0	4	30.812	61.429	-47.094	0.000	-8.736	-2.841
4	0	4	58.935	25.057	-25.057	0.000	-5.522	-1.846
4	0	4	82.906	88.970	-88.970	0.000	-12.193	-3.962
8	0	4	24.232	31.389	-88.200	0.000	-5.664	-1.842
8	0	4	30.536	28.282	31.389	0.000	-7.154	-2.326
1	0	4	135.675	139.195	-28.520	0.000	-3.354	-0.733
1	0	4	145.765	149.484	-19.719	0.000	-3.552	-1.155
1	0	4	22.941	19.466	-19.466	0.000	3.475	1.210
1	0	4	19.681	9.255	-19.466	0.000	1.130	0.390
1	0	4	38.101	39.240	-39.240	0.000	10.426	3.370
1	0	4	155.634	158.324	-158.324	0.000	-1.139	-0.375
1	0	4	127.777	133.301	-133.301	0.000	-2.591	-0.798
1	0	4	17.387	23.774	-23.774	0.000	-2.145	-0.698
1	0	4	229.745	276.566	-276.566	0.000	-4.787	-1.451
1	0	4	147.545	153.913	-153.913	0.000	-9.701	-2.970
1	0	4	46.742	54.716	-54.716	0.000	-2.373	-0.720
1	0	4	37.066	34.555	-34.555	0.000	-1.025	-0.323
1	0	4	106.339	107.394	-107.394	0.000	-1.425	-0.462
1	0	4	53.725	52.303	52.303	0.000	-1.025	-0.323
1	0	4	16.206	50.970	-50.970	0.000	-1.025	-0.323
1	0	4	26.200	14.814	-14.814	0.000	1.025	0.323
1	0	4	7.934	25.114	-25.114	0.000	1.025	0.323
1	0	4	17.930	2.668	-2.668	0.000	1.025	0.323
1	0	4	17.031	31.331	-31.331	0.000	13.303	4.376
1	0	4	134.139	149.076	-149.076	0.000	-16.588	-5.395
1	0	4	246.893	240.699	49.016	0.000	-10.175	-3.102
1	0	4	78.633	82.526	-82.526	0.000	-3.072	-1.006
1	0	4	92.626	97.726	-97.726	0.000	-5.072	-1.609
1	0	4	101.132	101.771	-101.771	0.000	-0.639	-0.203
1	0	4	102.424	99.778	99.778	0.000	-2.655	-0.823
1	0	4	12.711	52.388	-52.388	0.000	-10.116	-3.093
1	0	4	12.711	20.289	-20.289	0.000	-7.557	-2.458
1	0	4	68.699	39.999	-39.999	0.000	3.024	0.911
1	0	4	71.774	24.982	-24.982	0.000	6.477	2.146
1	0	4	41.430	85.537	-85.537	0.000	-4.107	-1.233
1	0	4	41.269	43.097	-43.097	0.000	-2.428	-0.770

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	25.357	24.652	54.652	0.0	-9.285	-3.019
1	1	0	25.754	25.528	55.528	0.0	-0.707	-0.707
1	1	0	25.754	25.618	30.618	0.0	-0.850	-0.850
1	1	0	25.310	25.071	58.071	0.0	-7.761	-2.524
1	1	0	45.974	45.974	16.664	0.0	0.000	1.349
1	1	0	45.974	46.064	46.064	0.0	0.000	0.000
1	1	0	157.141	157.141	21.120	0.0	0.000	1.922
1	1	0	157.141	157.572	134.402	0.0	2.738	0.890
1	1	0	35.549	34.570	34.570	0.0	0.979	0.655
1	1	0	35.549	101.644	101.644	0.0	2.014	0.318
1	1	0	125.047	122.849	101.644	0.0	-2.198	-2.782
1	1	0	75.003	72.510	72.510	0.0	0.000	0.672
1	1	0	40.008	44.771	42.510	0.0	0.811	0.811
1	1	0	38.501	37.444	37.444	0.0	0.000	0.063
1	1	0	55.268	55.963	37.444	0.0	-4.763	-1.549
1	1	0	29.768	31.793	31.793	0.0	0.000	0.344
1	1	0	51.816	48.622	48.622	0.0	-0.226	-0.226
1	1	0	28.537	27.311	27.311	0.0	-1.224	-1.039
1	1	0	85.766	86.570	59.922	0.0	-0.803	-0.695
1	1	0	45.373	46.273	187.038	0.0	0.900	0.261
1	1	0	175.161	171.742	171.742	0.0	-3.419	-2.347
1	1	0	14.299	17.840	17.840	0.0	3.541	1.112
1	1	0	19.411	172.319	172.319	0.0	2.909	0.546
1	1	0	73.896	79.640	79.640	0.0	5.744	1.868
1	1	0	16.790	4.002	4.002	0.0	-12.788	-4.159
1	1	0	103.879	102.885	102.885	0.0	-0.994	0.323
1	1	0	82.937	79.884	179.884	0.0	-3.053	0.993
1	1	0	87.796	91.553	91.553	0.0	3.757	1.222
1	1	0	24.017	22.000	22.000	0.0	-2.017	-0.656
1	1	0	152.036	159.513	159.513	0.0	7.477	2.431
1	1	0	151.017	45.486	45.486	0.0	-105.531	-1.825
1	1	0	120.516	120.288	120.288	0.0	-0.228	0.074
1	1	0	107.631	101.548	101.548	0.0	-6.083	1.979
1	1	0	44.006	50.958	50.958	0.0	6.952	-2.261
1	1	0	197.554	190.911	190.911	0.0	-6.643	-1.992
1	1	0	60.724	61.776	61.776	0.0	1.052	0.000
1	1	0	28.220	19.157	19.157	0.0	-9.063	0.359
1	1	0	179.496	123.636	123.636	0.0	-56.860	2.950
1	1	0	216.081	182.225	182.225	0.0	-34.856	0.976
1	1	0	212.022	219.293	219.293	0.0	7.271	0.821
1	1	0	210.526	206.049	206.049	0.0	-14.477	-1.051
1	1	0	116.395	212.559	212.559	0.0	96.164	1.246
1	1	0	82.414	116.395	116.395	0.0	34.981	0.661
1	1	0	25.555	93.696	93.696	0.0	68.141	0.180
1	1	0	74.173	21.784	21.784	0.0	-52.389	-3.069
1	1	0	28.139	77.653	77.653	0.0	49.514	1.152
1	1	0	70.513	24.856	24.856	0.0	-45.657	-1.432
1	1	0		69.659	69.659	0.0	0.000	0.278

Table 1 (cont)
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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
15	1	4	128.203	129.805	129.805	0.0	-1.601	-0.521
17	1	4	95.918	158.712	158.712	0.0	-4.266	-1.368
17	1	4	95.235	106.426	106.426	0.0	-7.191	-2.338
19	1	4	95.282	85.454	85.454	0.0	13.536	4.402
21	1	4	10.526	9.223	9.223	0.0	5.353	1.741
21	1	4	10.421	69.991	69.991	0.0	0.033	0.010
22	1	5	127.497	100.782	100.782	0.0	0.237	0.001
23	1	5	127.507	100.560	100.560	0.0	0.118	0.003
24	1	5	127.629	95.891	95.891	0.0	0.153	0.001
24	1	5	127.664	24.973	24.973	0.0	4.954	1.356
25	1	5	127.899	23.077	23.077	0.0	0.927	0.321
25	1	5	127.977	23.546	23.546	0.0	6.351	2.065
26	1	5	128.030	17.189	17.189	0.0	2.938	0.938
26	1	5	128.036	142.698	142.698	0.0	6.232	2.026
26	1	5	128.044	40.848	40.848	0.0	5.822	1.893
26	1	5	128.052	35.658	35.658	0.0	3.811	1.239
26	1	5	128.059	160.125	160.125	0.0	-0.585	-0.190
26	1	5	128.067	112.093	112.093	0.0	0.585	0.190
26	1	5	128.075	188.941	188.941	0.0	-1.644	-0.704
26	1	5	128.082	188.052	188.052	0.0	5.329	1.928
26	1	5	128.090	51.811	51.811	0.0	1.074	0.349
26	1	5	128.097	40.451	40.451	0.0	0.159	0.052
26	1	5	128.104	42.453	42.453	0.0	2.505	0.815
26	1	5	128.111	62.733	62.733	0.0	4.277	1.391
26	1	5	128.118	56.722	56.722	0.0	-2.069	-0.673
26	1	5	128.125	19.142	19.142	0.0	1.154	0.375
26	1	5	128.132	101.964	101.964	0.0	-1.638	-0.617
26	1	5	128.139	88.634	88.634	0.0	4.236	1.377
26	1	5	128.146	299.355	299.355	0.0	-1.226	-0.399
26	1	5	128.153	160.427	160.427	0.0	8.652	2.813
26	1	5	128.160	58.899	58.899	0.0	2.212	0.409
26	1	5	128.167	125.606	125.606	0.0	0.947	0.349
26	1	5	128.174	24.623	24.623	0.0	-16.274	-5.055
26	1	5	128.181	17.510	17.510	0.0	16.274	5.055
26	1	5	128.188	101.924	101.924	0.0	0.084	0.024
26	1	5	128.195	29.966	29.966	0.0	1.184	0.386
26	1	5	128.202	24.774	24.774	0.0	1.614	0.514
26	1	5	128.209	30.120	30.120	0.0	7.840	2.233
26	1	5	128.216	87.070	87.070	0.0	-1.234	-0.384
26	1	5	128.223	6.102	6.102	0.0	0.524	0.186
26	1	5	128.230	54.533	54.533	0.0	3.403	1.055
26	1	5	128.237	3.233	3.233	0.0	2.643	0.813
26	1	5	128.244	10.325	10.325	0.0	24.783	8.108
26	1	5	128.251	16.470	16.470	0.0	1.115	0.353
26	1	5	128.258	97.900	97.900	0.0	0.650	0.214
26	1	5	128.265	41.453	41.453	0.0	2.965	0.894
26	1	5	128.272	60.323	60.323	0.0	-0.142	-0.050
26	1	5	128.279	194.772	194.772	0.0	0.142	0.050
26	1	5	128.286	256.945	256.945	0.0	-7.851	-2.566
26	1	5	128.293	97.145	97.145	0.0	7.851	2.566
26	1	5	128.300	4.617	4.617	0.0	-0.040	-0.014
26	1	5	128.307	17.682	17.682	0.0	13.065	4.249

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

STRUCTURE FACTORS

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	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	10.306	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	8	8.733	18.435	247.445	0.0	3.734	1.214	*
1	1	8	194.504	180.628	18.438	0.0	9.876	-3.156	**
1	1	8	162.740	151.622	189.622	0.0	3.705	1.586	
1	1	8	164.214	161.222	151.622	0.0	-8.903	-2.895	
1	1	8	28.722	27.522	161.222	0.0	1.170	0.381	
1	1	8	59.156	56.728	-57.522	0.0	4.876	-1.586	
1	1	8	166.800	162.128	-56.728	0.0	4.630	1.505	
1	1	8	62.856	58.227	-192.227	0.0	14.644	4.762	
1	1	8	21.210	6.575	98.227	0.0	-0.267	0.087	
1	1	8	56.491	56.924	-59.227	0.0	7.085	2.304	*
1	1	8	121.060	121.378	-163.003	0.0	5.935	1.897	**
1	1	8	13.838	8.003	-49.003	0.0	3.131	1.018	*
1	1	8	59.918	93.009	-93.009	0.0	-12.062	-0.798	
1	1	8	7.842	19.974	-19.974	0.0	11.448	3.723	
1	1	8	178.974	181.420	-181.420	0.0	8.747	2.845	
1	1	8	26.692	15.226	-23.226	0.0	-7.101	-2.309	
1	1	9	32.043	50.226	-50.226	0.0	4.323	1.308	
1	1	9	43.145	126.334	126.334	0.0	-4.529	-0.064	
1	1	9	130.356	36.722	-36.722	0.0	0.156	1.916	
1	1	9	32.166	98.725	-98.725	0.0	-2.720	-2.568	
1	1	9	107.233	67.053	29.053	0.0	3.265	3.013	
1	1	9	34.965	29.053	75.952	0.0	5.785	1.752	
1	1	9	66.823	75.952	32.957	0.0	3.511	0.816	
1	1	9	41.361	32.957	30.274	0.0	-4.121	-0.407	
1	1	9	32.280	30.274	74.781	0.0	-1.457	-0.474	
1	1	9	80.169	74.781	-23.175	0.0	3.867	5.250	
1	1	9	25.616	23.175	61.423	0.0	-1.801	-0.645	
1	1	9	63.933	61.423	-44.580	0.0	17.435	3.850	
1	1	9	43.328	80.907	80.907	0.0	5.964	1.839	
1	1	9	95.028	74.154	-74.154	0.0	-1.679	-1.426	
1	1	10	72.997	74.154	80.523	0.0	4.598	1.426	
1	1	10	78.632	80.523	-23.227	0.0	-0.056	-0.017	
1	1	10	27.400	23.423	77.952	0.0	1.679	1.426	
1	1	10	23.310	77.952	113.209	0.0	4.598	1.426	
1	1	10	55.870	11.532	-59.906	0.0	0.544	0.177	
1	1	10	114.888	113.209	113.209	0.0	0.0	0.0	
1	1	10	83.767	79.170	24.170	0.0	0.0	0.0	
1	1	10	24.786	24.170	24.170	0.0	0.0	0.0	

Table 2 (cont)
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H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA/SIGMA
13	1	10	50.135	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	3.335	4.179	-28.179	0.0	-6.715	-2.184
8	1	11	72.885	61.993	-66.993	0.0	-7.730	-2.514
10	1	11	68.089	84.402	84.402	0.0	-4.818	-1.567
12	1	11	15.718	17.802	61.805	0.0	0.293	0.092
14	1	11	40.008	38.038	-18.022	0.0	-0.304	-0.099
16	1	11	152.190	40.252	140.252	0.0	1.970	0.641
18	1	11	22.941	137.072	-137.072	0.0	0.270	0.070
20	1	11	25.278	22.026	-133.728	0.0	8.432	2.742
22	1	12	51.017	55.688	-22.026	0.0	-0.134	-0.044
24	1	12	27.402	22.830	-55.688	0.0	3.011	0.979
26	1	12	27.215	19.919	-22.830	0.0	-4.811	-1.584
28	1	12	40.162	36.885	-19.850	0.0	0.572	0.186
30	1	12	72.851	69.552	-36.885	0.0	7.297	2.373
32	1	12	19.466	5.895	-69.552	0.0	3.299	1.065
34	1	12	77.064	83.338	-83.338	0.0	13.570	4.413
36	1	12	22.971	33.514	-33.514	0.0	-16.217	-5.041
38	1	12	11.128	75.671	-75.671	0.0	-4.342	-1.477
40	1	12	17.224	33.235	33.235	0.0	-22.011	-7.158
42	1	12	66.085	22.564	-22.564	0.0	-15.184	-4.938
44	1	12	30.505	61.883	-61.883	0.0	4.502	1.367
46	1	13	11.132	16.446	-33.480	0.0	-2.574	-0.967
48	1	13	53.692	68.217	16.446	0.0	5.314	1.728
50	1	13	59.468	66.020	-66.020	0.0	-14.324	-4.723
52	1	13	107.046	55.400	65.400	0.0	13.448	4.121
54	1	13	24.355	100.948	100.948	0.0	6.598	1.983
56	1	13	105.540	108.571	-19.821	0.0	7.035	2.147
58	1	13	95.238	105.165	-108.571	0.0	-3.027	-0.986
60	1	13	42.858	57.195	57.195	0.0	-14.208	-4.228
62	1	14	46.250	50.457	50.457	0.0	14.207	4.650
64	1	14	36.815	82.754	82.754	0.0	-10.247	-3.368
66	1	14	196.995	38.501	38.501	0.0	-11.686	-3.210
68	1	14	44.621	197.663	197.663	0.0	-4.415	-1.436
70	1	14	40.995	49.035	-31.769	0.0	3.216	0.949
72	1	14	45.257	48.707	-48.707	0.0	-3.115	-1.049
74	1	14	14.392	39.841	-39.841	0.0	5.456	1.714
76	1	14	104.371	6.065	6.065	0.0	8.337	2.714
78	1	14	70.298	105.639	-105.639	0.0	-3.152	-1.042
80	1	15	49.172	71.430	-71.430	0.0	3.132	1.042
82	1	15	36.898	54.720	-54.720	0.0	-1.804	-0.574
84	1	15	71.859	99.277	99.277	0.0	-0.809	-0.243
86	1	15	14.453	32.658	-32.658	0.0	-5.285	-1.719
88	1	15	19.738	19.738	19.738	0.0	-5.285	-1.719

Table 2 (cont)
PAGE 30-8

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	34.779	29.058	29.058	0.0	-4.571	-1.486
0	1	1	37.087	31.058	31.058	0.0	-6.029	-2.149
0	1	1	37.922	32.778	-29.278	0.0	3.447	1.186
0	1	1	41.522	37.972	-17.022	0.0	3.060	1.057
0	1	1	55.074	34.831	34.831	0.0	-3.233	-1.076
0	1	1	112.000	187.023	187.023	0.0	-9.555	-3.042
0	1	1	33.424	129.473	-129.473	0.0	0.101	0.130
0	1	1	33.550	36.952	-36.952	0.0	3.375	1.106
0	1	1	122.422	29.598	29.598	0.0	-10.378	-3.375
0	1	1	122.913	130.588	130.588	0.0	-9.166	-2.655
0	1	1	52.155	43.632	14.322	0.0	0.281	0.091
0	1	1	13.684	61.161	-61.161	0.0	-9.006	-2.929
0	1	1	40.008	34.895	4.008	0.0	0.365	0.119
0	1	1	22.541	27.892	-27.892	0.0	5.112	1.663
0	1	1	159.416	167.115	-167.115	0.0	-7.699	-2.504
0	1	1	64.978	64.794	0.184	0.0	-0.194	0.060
0	1	1	172.470	178.445	-178.445	0.0	4.575	1.618
0	1	1	122.084	132.862	-132.862	0.0	0.178	0.060
0	1	1	97.320	105.636	-105.636	0.0	-4.575	-1.618
0	1	1	105.177	118.054	-118.054	0.0	12.583	4.189
0	1	1	19.835	35.334	-35.334	0.0	3.501	1.138
0	1	1	40.346	35.698	4.648	0.0	-4.548	-1.512
0	1	1	186.416	186.700	-284.287	0.0	0.284	0.092
0	1	1	201.260	214.327	-214.327	0.0	-13.058	-4.246
0	1	1	61.688	58.264	3.424	0.0	3.423	1.113
0	1	1	229.838	249.833	-249.833	0.0	-19.395	-6.502
0	1	1	38.624	36.418	2.206	0.0	-2.206	-0.718
0	1	1	66.854	72.696	-72.696	0.0	5.842	1.900
0	1	1	25.585	24.882	0.703	0.0	1.070	0.348
0	1	1	78.417	77.347	1.070	0.0	-0.347	-0.120
0	1	1	41.238	41.878	-64.641	0.0	0.641	0.208
0	1	1	80.600	85.814	-85.814	0.0	0.311	0.100
0	1	1	16.514	24.637	-24.637	0.0	8.127	2.641
0	1	1	176.418	176.629	-76.629	0.0	0.211	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	88.565	88.441	0.124	0.0	-0.124	-0.040
0	1	1	57.106	56.230	0.876	0.0	0.875	0.285
0	1	1	60.488	66.823	-66.823	0.0	0.334	0.100
0	1	1	209.788	209.049	0.739	0.0	0.739	0.240
0	1	1	17.774	16.585	1.189	0.0	1.190	0.387
0	1	1	43.083	38.821	5.262	0.0	4.262	1.386
0	1	1	70.422	68.265	2.157	0.0	2.157	0.717
0	1	1	94.961	97.689	-97.689	0.0	2.728	0.897
0	1	1	155.542	167.818	-167.818	0.0	-12.276	-3.897
0	1	1	80.282	176.414	-176.414	0.0	3.879	1.232
0	1	1	55.261	61.597	-61.597	0.0	-6.336	-2.061
0	1	1	78.078	73.655	4.424	0.0	-4.424	-1.439

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	1	N	40.715	43.480	-43.480	0.0	-2.765	-0.899
1	1	N	52.139	78.689	-78.689	0.0	-2.765	-0.899
1	1	N	52.139	13.104	-13.104	0.0	-2.765	-0.899
1	1	N	52.139	48.867	-48.867	0.0	-2.765	-0.899
1	1	N	52.139	30.898	-30.898	0.0	-2.765	-0.899
1	1	N	21.521	16.831	-16.831	0.0	-2.765	-0.899
1	1	N	21.521	221.943	-221.943	0.0	-2.765	-0.899
1	1	N	15.572	15.508	-15.508	0.0	-2.765	-0.899
1	1	N	15.572	123.905	-123.905	0.0	-2.765	-0.899
1	1	N	15.572	18.881	-18.881	0.0	-2.765	-0.899
1	1	N	39.052	18.988	-18.988	0.0	-2.765	-0.899
1	1	N	19.052	92.895	-92.895	0.0	-2.765	-0.899
1	1	N	44.074	124.707	-124.707	0.0	-2.765	-0.899
1	1	N	129.587	124.707	-124.707	0.0	-2.765	-0.899
1	1	N	139.597	142.125	-142.125	0.0	-2.765	-0.899
1	1	N	15.899	26.829	-26.829	0.0	-2.765	-0.899
1	1	N	15.899	68.829	-68.829	0.0	-2.765	-0.899
1	1	N	17.315	70.829	-70.829	0.0	-2.765	-0.899
1	1	N	17.315	140.710	-140.710	0.0	-2.765	-0.899
1	1	N	175.680	179.479	-179.479	0.0	-2.765	-0.899
1	1	N	209.664	206.463	-206.463	0.0	-2.765	-0.899
1	1	N	116.918	110.110	-110.110	0.0	-2.765	-0.899
1	1	N	40.100	42.889	-42.889	0.0	-2.765	-0.899
1	1	N	50.494	55.262	-55.262	0.0	-2.765	-0.899
1	1	N	29.138	20.459	-20.459	0.0	-2.765	-0.899
1	1	N	79.923	81.577	-81.577	0.0	-2.765	-0.899
1	1	N	95.545	107.054	-107.054	0.0	-2.765	-0.899
1	1	N	100.558	107.054	-107.054	0.0	-2.765	-0.899
1	1	N	37.640	38.617	-38.617	0.0	-2.765	-0.899
1	1	N	99.604	93.277	-93.277	0.0	-2.765	-0.899
1	1	N	16.606	17.789	-17.789	0.0	-2.765	-0.899
1	1	N	16.606	92.637	-92.637	0.0	-2.765	-0.899
1	1	N	73.773	74.731	-74.731	0.0	-2.765	-0.899
1	1	N	14.063	19.622	-19.622	0.0	-2.765	-0.899
1	1	N	46.600	41.539	-41.539	0.0	-2.765	-0.899
1	1	N	59.935	19.181	-19.181	0.0	-2.765	-0.899
1	1	N	187.093	50.357	-50.357	0.0	-2.765	-0.899
1	1	N	183.467	183.677	-183.677	0.0	-2.765	-0.899
1	1	N	221.350	184.817	-184.817	0.0	-2.765	-0.899
1	1	N	14.954	198.523	-198.523	0.0	-2.765	-0.899
1	1	N	22.541	21.617	-21.617	0.0	-2.765	-0.899
1	1	N	241.369	237.235	-237.235	0.0	-2.765	-0.899
1	1	N	179.954	80.703	-80.703	0.0	-2.765	-0.899
1	1	N	113.135	115.021	-115.021	0.0	-2.765	-0.899
1	1	N	62.212	57.177	-57.177	0.0	-2.765	-0.899

STRUCTURE FACTORS
DELTA/SIGMA

DELTA F

A(CALC)

B(CALC)

F(OBS)

F(CALC)

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

Table 2 (Cont)
PAGE#10

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
11	2	5	53.692	53.518	53.518	0.000	0.174	0.057
12	2	5	37.342	37.342	-37.342	0.000	-2.896	-0.932
13	2	5	22.924	22.924	-22.924	0.000	-1.876	-0.610
14	2	5	43.821	43.821	43.821	0.000	0.278	0.091
15	2	5	17.802	17.802	17.802	0.000	-6.335	-2.060
16	2	5	11.811	11.811	11.811	0.000	-10.955	-3.465
17	2	5	28.877	28.877	-28.877	0.000	-17.714	-5.760
18	2	5	40.064	40.064	-40.064	0.000	-9.538	-3.232
19	2	5	90.994	90.994	-90.994	0.000	-3.866	-1.257
20	2	5	89.149	89.149	-89.149	0.000	0.299	0.088
21	2	5	66.577	66.577	-66.577	0.000	-2.303	-0.749
22	2	5	172.240	172.240	-172.240	0.000	-4.448	-1.447
23	2	5	63.180	63.180	-63.180	0.000	-5.772	-1.877
24	2	5	141.115	141.115	-141.115	0.000	-1.975	-0.642
25	2	5	57.629	57.629	-57.629	0.000	-1.514	-0.590
26	2	5	127.024	127.024	-127.024	0.000	1.178	0.383
27	2	5	27.123	27.123	27.123	0.000	4.093	1.331
28	2	5	135.524	135.524	-135.524	0.000	-3.376	-1.098
29	2	5	136.660	136.660	-136.660	0.000	-0.261	-0.085
30	2	5	5.781	5.781	-5.781	0.000	0.457	0.147
31	2	5	5.938	5.938	-5.938	0.000	-0.017	-0.006
32	2	5	15.403	15.403	-15.403	0.000	-19.077	-5.173
33	2	5	3.475	3.475	3.475	0.000	-0.457	-0.147
34	2	5	30.094	30.094	-30.094	0.000	-1.273	-0.430
35	2	5	75.526	75.526	-75.526	0.000	2.426	0.882
36	2	5	53.016	53.016	-53.016	0.000	-0.429	-0.132
37	2	5	29.522	29.522	-29.522	0.000	0.429	0.132
38	2	5	45.789	45.789	-45.789	0.000	-0.429	-0.132
39	2	5	186.416	186.416	-186.416	0.000	-2.564	-0.835
40	2	5	39.977	39.977	-39.977	0.000	0.564	0.182
41	2	5	13.408	13.408	-13.408	0.000	5.226	1.682
42	2	5	15.323	15.323	-15.323	0.000	7.327	2.200
43	2	5	18.444	18.444	-18.444	0.000	3.271	1.064
44	2	5	12.485	12.485	-12.485	0.000	0.051	0.016
45	2	5	52.432	52.432	-52.432	0.000	4.095	1.302
46	2	5	80.934	80.934	-80.934	0.000	4.275	1.350
47	2	5	130.049	127.201	-127.201	0.000	2.848	0.920
48	2	5	134.800	137.925	-137.925	0.000	-3.325	-1.056
49	2	5	139.789	102.234	-102.234	0.000	-2.445	-0.792
50	2	5	10.389	170.907	-170.907	0.000	-3.082	-1.007
51	2	5	63.318	64.321	-64.321	0.000	-1.007	-0.320
52	2	5	20.880	19.366	-19.366	0.000	1.514	0.490
53	2	5	33.454	90.362	-90.362	0.000	3.024	1.005
54	2	5	31.134	31.134	-31.134	0.000	0.726	0.239
55	2	5	89.737	89.737	-89.737	0.000	67.341	2.087
56	2	5	55.955	55.955	-55.955	0.000	-2.965	-0.964
57	2	5	70.320	75.335	-75.335	0.000	-3.504	-1.139
58	2	5	112.819	112.819	-112.819	0.000	1.514	0.427
59	2	5	101.848	101.848	-101.848	0.000	-2.707	-0.888
60	2	5	116.113	116.113	-116.113	0.000	-0.408	-0.132
61	2	5	130.077	126.102	-126.102	0.000	-3.316	-1.078
62	2	5	24.571	13.416	-13.416	0.000	1.155	0.367

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	123.808	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	95.163	52.541	0.0	0.0	2.621	0.852
0	0	0	21.437	77.437	0.0	0.0	1.902	0.618
0	0	0	11.378	11.620	0.0	0.0	0.242	0.081
0	0	0	29.685	25.952	0.0	0.0	3.733	1.177
0	0	0	38.470	46.707	0.0	0.0	-2.038	-0.672
0	0	0	26.639	34.085	0.0	0.0	3.417	1.144
0	0	0	26.539	34.085	0.0	0.0	3.546	1.134
0	0	0	37.720	27.504	0.0	0.0	-3.216	-0.974
0	0	0	37.721	27.504	0.0	0.0	-3.216	-0.974
0	0	0	37.721	30.137	0.0	0.0	-0.584	-0.170
0	0	0	183.987	0.444	0.0	0.0	-0.543	-0.158
0	0	0	24.048	186.457	0.0	0.0	2.409	0.703
0	0	0	198.932	22.945	0.0	0.0	-2.471	-0.703
0	0	0	15.437	194.645	0.0	0.0	1.203	0.359
0	0	0	24.632	29.479	0.0	0.0	4.843	1.393
0	0	0	20.245	30.494	0.0	0.0	-14.022	-4.566
0	0	0	47.777	21.015	0.0	0.0	-15.862	-4.566
0	0	0	67.561	34.205	0.0	0.0	8.351	2.377
0	0	0	67.715	64.953	0.0	0.0	2.762	0.848
0	0	0	25.278	66.773	0.0	0.0	4.495	1.271
0	0	0	137.429	35.470	0.0	0.0	-10.142	-2.914
0	0	0	119.716	147.732	0.0	0.0	-2.828	-0.822
0	0	0	44.805	121.322	0.0	0.0	-3.523	-1.061
0	0	0	55.901	48.068	0.0	0.0	-1.836	-0.522
0	0	0	45.621	59.261	0.0	0.0	-6.640	-1.861
0	0	0	8.764	47.989	0.0	0.0	-1.308	-0.425
0	0	0	54.907	4.352	0.0	0.0	4.943	1.435
0	0	0	72.881	56.907	0.0	0.0	-1.977	-0.605
0	0	0	45.820	78.025	0.0	0.0	-5.203	-1.473
0	0	0	77.463	46.303	0.0	0.0	-3.163	-0.917
0	0	0	131.309	72.709	0.0	0.0	-4.584	-1.346
0	0	0	77.187	132.588	0.0	0.0	-1.678	-0.416
0	0	0	50.156	170.248	0.0	0.0	6.929	2.256
0	0	0	48.834	48.794	0.0	0.0	0.060	0.017
0	0	0	11.870	15.446	0.0	0.0	-3.576	-1.013
0	0	0	30.075	8.489	0.0	0.0	2.586	0.766
0	0	0	49.112	25.997	0.0	0.0	-2.109	-0.602
0	0	0	99.112	48.214	0.0	0.0	-1.375	-0.402
0	0	0	15.038	101.905	0.0	0.0	-3.539	-1.013
0	0	0	18.937	34.377	0.0	0.0	-5.479	-1.581
0	0	0	18.451	20.535	0.0	0.0	-3.079	-0.894
0	0	0	69.622	25.459	0.0	0.0	8.169	2.317
0	0	0	37.117	10.402	0.0	0.0	-6.283	-1.786
0	0	0	11.563	37.065	0.0	0.0	-7.502	-2.142
0	0	0	41.330	15.005	0.0	0.0	-0.833	-0.271
0	0	0	40.477	40.477	0.0	0.0	0.000	0.000

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	-0.011	-0.011	
1	1	1	18.286	97.496	-30.226	0.0	0.241	0.241	
1	1	1	18.286	70.226	-76.826	0.0	-1.566	-1.566	
1	1	1	18.286	120.826	132.994	0.0	-4.068	-4.068	
1	1	1	17.070	12.994	-72.121	0.0	-2.894	-2.894	
1	1	1	17.070	28.286	25.985	0.0	-1.546	-1.546	
1	1	1	17.070	48.646	-8.646	0.0	-8.980	-8.980	**
1	1	1	18.286	8.646	-43.646	0.0	12.450	12.450	**
1	1	1	18.286	8.322	-8.422	0.0	3.157	3.157	**
1	1	1	17.070	2.922	8.322	0.0	0.942	0.942	**
1	1	1	17.070	40.121	2.922	0.0	1.648	1.648	**
1	1	1	36.902	55.121	40.121	0.0	-1.061	-1.061	
1	1	1	33.529	32.388	55.388	0.0	-2.892	-2.892	**
1	1	1	33.529	20.529	32.388	0.0	-0.937	-0.937	**
1	1	1	195.180	207.529	207.529	0.0	-4.024	-4.024	**
1	1	1	22.264	20.315	20.315	0.0	0.634	0.634	**
1	1	1	95.364	37.427	-37.427	0.0	-1.185	-1.185	**
1	1	1	21.618	8.303	-37.427	0.0	1.566	1.566	**
1	1	1	149.484	155.601	155.601	0.0	-4.330	-4.330	**
1	1	1	85.212	186.671	186.671	0.0	-1.989	-1.989	**
1	1	1	131.555	18.447	-18.447	0.0	0.474	0.474	**
1	1	1	109.199	138.820	-138.820	0.0	-2.634	-2.634	**
1	1	1	32.781	107.757	-107.757	0.0	2.362	2.362	**
1	1	1	30.875	9.059	19.059	0.0	0.470	0.470	**
1	1	1	106.647	113.648	-22.728	0.0	4.487	4.487	**
1	1	1	41.515	40.154	-140.354	0.0	4.607	4.607	**
1	1	1	60.827	54.553	-64.553	0.0	2.633	2.633	**
1	1	1	97.131	68.003	-68.003	0.0	-2.277	-2.277	**
1	1	1	23.648	28.617	-28.617	0.0	0.442	0.442	**
1	1	1	45.205	41.219	-41.219	0.0	-1.212	-1.212	**
1	1	1	66.577	66.755	-66.755	0.0	0.284	0.284	**
1	1	1	130.594	140.722	140.722	0.0	-1.616	-1.616	**
1	1	1	27.051	27.923	-27.923	0.0	1.296	1.296	**
1	1	1	40.521	38.433	-38.433	0.0	-0.061	-0.061	**
1	1	1	122.084	125.911	125.911	0.0	3.254	3.254	**
1	1	1	150.002	52.259	52.259	0.0	-0.300	-0.300	**
1	1	1	7.934	11.250	11.250	0.0	-1.244	-1.244	**
1	1	1	35.764	45.112	-45.112	0.0	1.078	1.078	**
1	1	1	120.320	252.914	252.914	0.0	-3.056	-3.056	**
1	1	1	12.222	124.722	124.722	0.0	-9.607	-9.607	**
1	1	1	51.222	56.806	56.806	0.0	-1.471	-1.471	**
1	1	1	212.678	238.884	238.884	0.0	1.813	1.813	**
1	1	1	99.856	97.503	-97.503	0.0	-2.487	-2.487	**
1	1	1	11.101	9.713	9.713	0.0	2.452	2.452	**
1	1	1	78.078	86.557	-86.557	0.0	-0.470	-0.470	**
1	1	1	55.783	57.935	57.935	0.0	0.700	0.700	**
1	1	1	22.756	9.077	-9.077	0.0	-0.128	-0.128	**
1	1	1	198.524	198.977	198.977	0.0	-0.456	-0.456	**
1	1	1	13.131	16.687	16.687	0.0	-1.157	-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	-291.566	0.00	-29.778	-9.683	*
4	6	1	250.774	289.506	-289.506	0.00	-5.656	-1.839	*
0	0	0	250.774	289.506	-289.506	0.00	-25.825	-8.398	*
0	0	0	75.118	84.984	-84.984	0.00	-4.932	-1.601	
0	0	0	234.680	242.480	-242.480	0.00	-7.599	-2.471	
0	0	0	121.570	122.775	-122.775	0.00	-2.030	-0.678	
0	0	0	94.321	97.050	-97.050	0.00	-1.254	-0.421	
0	0	0	23.371	31.643	-31.643	0.00	-5.759	-1.863	
4	4	1	11.378	20.822	-20.822	0.00	-4.854	-1.578	
1	1	1	5.359	45.852	-45.852	0.00	-3.690	-1.186	
1	1	1	9.918	101.095	-101.095	0.00	-9.294	-2.822	*
1	1	1	102.157	81.793	101.793	0.00	8.517	2.770	*
1	1	1	84.874	97.310	-97.310	0.00	-2.044	-0.665	*
1	1	1	91.855	81.953	81.953	0.00	5.123	1.666	*
1	1	1	92.210	93.557	-93.557	0.00	4.847	1.576	*
1	1	1	49.172	61.420	-61.420	0.00	2.951	0.950	
1	1	1	37.025	53.375	-53.375	0.00	-0.790	-0.257	
1	1	1	101.757	36.202	36.202	0.00	-4.163	-1.354	
1	1	1	55.378	102.202	-102.202	0.00	0.813	0.264	
1	1	1	34.907	96.392	-96.392	0.00	-0.449	-0.146	
1	1	1	53.723	60.400	-60.400	0.00	1.348	0.406	
1	1	1	91.629	34.400	34.400	0.00	-0.754	-0.258	
1	1	1	30.413	49.512	-49.512	0.00	4.533	1.376	
1	1	1	25.124	28.123	-28.123	0.00	-4.503	-1.594	
1	1	1	39.977	22.777	22.777	0.00	-2.347	-0.722	
1	1	1	113.904	43.134	43.134	0.00	-3.157	-0.963	
1	1	1	175.959	118.541	-118.541	0.00	-4.637	-1.508	
1	1	1	31.028	22.930	22.930	0.00	-0.280	-0.086	
1	1	1	16.421	22.964	-22.964	0.00	1.729	0.562	*
1	1	1	26.938	6.095	-6.095	0.00	10.412	3.386	*
1	1	1	79.897	30.511	30.511	0.00	-8.347	-2.910	*
1	1	1	80.938	82.773	-82.773	0.00	-4.156	-1.352	*
1	1	1	4.520	12.533	-12.533	0.00	-7.433	-2.599	*
1	1	1	53.723	50.055	-50.055	0.00	3.430	1.186	*
1	1	1	64.066	55.696	-55.696	0.00	0.750	0.278	*
1	1	1	113.955	113.955	0.00	0.00	0.00	0.00	*
1	1	1	119.122	119.912	-119.912	0.00	0.789	0.257	*
1	1	1	14.014	4.199	4.199	0.00	-2.886	-1.215	*
1	1	1	129.614	24.950	24.950	0.00	-4.663	-1.516	*
1	1	1	103.571	110.216	-110.216	0.00	0.044	-0.161	*
1	1	1	43.022	43.096	-43.096	0.00	-3.289	-1.014	*
1	1	1	28.445	30.744	-30.744	0.00	-1.528	-0.478	*
1	1	1	91.353	89.278	-89.278	0.00	-1.528	-0.478	*
1	1	1	66.069	68.167	-68.167	0.00	-0.160	-0.052	*
1	1	1	11.132	11.766	-11.766	0.00	8.587	2.792	*
1	1	1	14.509	24.549	-24.549	0.00	0.160	0.052	*
1	1	1	119.778	111.191	-111.191	0.00	8.587	2.792	*

Table 2 (cont)
PAGE#14

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA	STRUCTURE FACTORS
-18	3	3	55.753	57.825	-57.825	0.0	-2.072	-0.674	
-20	3	3	100.670	100.612	-100.612	0.0	3.342	3.342	
-1	3	3	108.337	84.871	-84.871	0.0	-3.164	-1.029	
-	4	4	70.328	108.792	-108.792	0.0	9.541	3.103	
-	4	4	10.281	55.035	55.035	0.0	1.302	0.423	
-	4	4	168.519	97.530	68.530	0.0	2.998	0.575	
-	4	4	106.652	173.233	173.233	0.0	-5.047	-0.666	
-	4	4	48.895	20.541	-20.541	0.0	3.076	1.000	
-	4	4	19.743	170.591	-170.591	0.0	5.189	1.687	
-	4	4	31.490	32.137	-32.137	0.0	-3.242	-1.493	
-	4	4	29.829	18.918	-18.918	0.0	0.885	0.268	
-	4	4	56.429	30.423	-30.423	0.0	1.066	0.347	
-	4	4	45.420	57.514	57.514	0.0	1.179	0.179	
-	4	4	33.273	44.076	44.076	0.0	-1.085	-0.353	
-	4	4	88.872	29.009	-29.009	0.0	1.344	0.437	
-	4	4	19.281	80.271	80.271	0.0	4.265	1.387	
-	4	4	59.702	19.443	-19.443	0.0	8.601	2.797	**
-	4	4	123.803	88.720	-88.720	0.0	0.920	0.320	
-	4	4	156.318	125.837	-125.837	0.0	3.966	1.290	
-	4	4	260.927	198.510	-198.510	0.0	-2.192	-0.713	
-	4	4	108.030	255.101	-255.101	0.0	5.826	1.895	
-	4	4	47.173	106.755	106.755	0.0	1.275	0.415	
-	4	4	33.150	51.433	51.433	0.0	-4.262	-1.386	
-	4	4	161.723	25.943	-25.943	0.0	7.507	2.344	
-	4	4	106.185	163.084	163.084	0.0	-1.431	-0.443	
-	4	4	59.597	101.172	-101.172	0.0	5.013	1.630	
-	4	4	4.828	58.969	-58.969	0.0	0.528	0.204	**
-	4	4	22.110	13.613	-13.613	0.0	-8.785	-2.857	**
-	4	4	87.150	19.855	-19.855	0.0	2.233	0.733	
-	4	4	17.375	85.157	85.157	0.0	1.993	0.648	
-	4	4	20.265	75.055	75.055	0.0	-0.544	-0.177	**
-	4	4	59.966	23.707	-23.707	0.0	19.215	3.322	**
-	4	4	18.881	60.434	-60.434	0.0	-3.441	-1.119	**
-	4	4	19.835	15.316	-15.316	0.0	-5.599	-0.152	**
-	4	4	62.026	29.320	-29.320	0.0	3.800	1.160	
-	4	4	60.796	23.972	-23.972	0.0	-3.437	-1.245	
-	4	4	49.787	59.169	-59.169	0.0	2.457	0.929	
-	4	4	24.694	160.518	-160.518	0.0	6.087	2.012	
-	4	4	26.293	67.107	-67.107	0.0	-0.349	-0.215	
-	4	4	25.801	50.756	-50.756	0.0	5.711	2.052	
-	4	4	13.162	29.737	-29.737	0.0	-0.640	-0.215	
-	4	4	67.838	25.681	-25.681	0.0	5.107	1.640	
-	4	4	68.602	19.694	-19.694	0.0	-0.412	-0.140	**
-	4	4	68.914	15.355	-15.355	0.0	-0.803	-0.271	**
-	4	4	40.469	68.641	-68.641	0.0	-0.229	-0.083	**
-	4	4	45.851	28.831	-28.831	0.0	-0.826	-0.305	**
-	4	4		69.841	69.841	0.0	-0.858	-0.301	**
-	4	4		41.327	-41.327	0.0	-0.858	-0.301	**
-	4	4		46.491	-46.491	0.0	-0.203	-0.070	**

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
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	0	0	110.152	109.475	-109.475	0.0	0.677	0.220	
0	0	0	67.500	65.047	-65.047	0.0	2.453	0.803	
0	0	0	94.254	91.427	-91.427	0.0	2.827	0.976	
0	0	0	92.716	81.308	-81.308	0.0	1.209	0.419	
0	0	0	89.411	117.144	117.144	0.0	2.733	0.910	
1	0	0	119.562	148.500	148.500	0.0	2.938	0.986	
1	0	0	44.897	70.637	70.637	0.0	-3.740	-1.171	
1	1	1	151.944	149.941	-149.941	0.0	1.598	0.500	
1	1	1	51.816	47.677	-47.677	0.0	2.003	0.651	
1	1	1	24.171	21.063	-21.063	0.0	4.140	1.346	
1	1	1	77.525	76.692	-76.692	0.0	3.108	1.011	
1	1	1	54.369	60.515	-60.515	0.0	0.829	0.270	
1	1	1	73.835	67.794	-67.794	0.0	6.047	1.999	
1	1	1	37.117	27.136	-27.136	0.0	6.041	1.964	
1	1	1	71.282	75.647	75.647	0.0	9.981	3.246	
1	1	1	155.572	152.889	-152.889	0.0	2.685	0.873	
1	1	1	34.473	31.264	-31.264	0.0	3.158	1.059	
1	1	1	33.704	32.493	-32.493	0.0	1.237	0.409	*
1	1	1	32.255	27.492	-27.492	0.0	2.451	0.801	*
1	1	1	91.027	88.262	-88.262	0.0	2.766	0.898	
1	1	1	86.258	80.657	-80.657	0.0	7.601	2.426	
1	1	1	14.361	2.101	-2.101	0.0	12.260	3.987	*
1	1	1	58.520	56.666	-56.666	0.0	1.854	0.603	
1	1	1	43.331	44.778	44.778	0.0	-1.447	-0.452	
1	1	1	30.025	35.511	35.511	0.0	-5.486	-1.768	
1	1	1	106.023	105.044	-105.044	0.0	0.976	0.338	
1	1	1	156.033	160.938	160.938	0.0	-4.908	-1.505	
2	0	0	21.220	22.289	22.289	0.0	-1.069	-0.328	
2	0	0	147.044	144.345	-144.345	0.0	2.679	0.881	
2	0	0	91.928	94.131	94.131	0.0	-2.203	-0.700	
2	0	0	89.825	88.377	-88.377	0.0	1.472	0.471	
2	0	0	98.347	94.209	-94.209	0.0	4.134	1.344	
2	0	0	75.927	75.526	-75.526	0.0	0.401	0.150	
2	0	0	154.855	151.609	-151.609	0.0	3.247	1.059	
2	0	0	166.151	162.745	-162.745	0.0	3.404	1.124	
2	0	0	11.685	16.520	16.520	0.0	-4.835	-1.551	*
2	0	0	73.855	74.583	74.583	0.0	-0.728	-0.249	*
2	0	0	71.685	68.535	-68.535	0.0	3.054	0.979	*
2	0	0	80.652	78.499	-78.499	0.0	2.163	0.715	
2	0	0	23.994	16.395	-16.395	0.0	7.593	2.459	*
2	0	0	13.315	10.981	-10.981	0.0	12.334	3.911	*
2	0	0	43.052	42.866	-42.866	0.0	0.186	0.062	*
2	0	0	130.088	130.601	130.601	0.0	-0.514	-0.172	*
2	0	0	130.049	130.601	130.601	0.0	-0.553	-0.180	*
2	0	0	21.987	23.772	23.772	0.0	-1.785	-0.580	
2	0	0	90.933	86.769	-86.769	0.0	4.163	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	-1.284	**
1	0	0	115.294	104.093	104.093	0.0	11.201	1.344	*
1	0	0	24.540	113.633	-13.147	0.0	11.333	3.705	*
1	0	0	37.979	18.147	38.200	0.0	-0.229	-0.074	*
1	0	0	76.541	58.320	-77.861	0.0	-1.330	-1.0429	*
1	0	0	54.917	77.861	-68.881	0.0	-3.744	-1.224	*
1	0	0	55.650	47.821	47.821	0.0	-2.532	-1.0823	*
1	0	0	16.102	7.102	-47.195	0.0	9.780	3.550	**
1	0	0	58.520	5.443	-55.425	0.0	-3.951	-1.087	*
1	0	0	47.091	40.492	-30.425	0.0	3.333	1.088	*
1	0	0	41.259	67.492	-57.422	0.0	0.271	0.083	*
1	0	0	72.543	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	16.146	0.0	-0.699	-0.227	*
1	0	0	54.707	50.822	-50.822	0.0	5.146	1.674	*
1	0	0	82.860	57.170	57.170	0.0	-4.731	-1.558	*
1	0	0	22.049	7.085	-70.128	0.0	2.472	-0.804	*
1	0	0	34.592	7.085	-7.085	0.0	4.573	1.548	*
1	0	0	55.890	94.003	-94.003	0.0	14.063	4.573	*
1	0	0	8.118	53.523	-60.232	0.0	0.721	0.221	*
1	0	0	22.101	19.594	-19.594	0.0	3.377	1.098	*
1	0	0	94.121	94.121	94.121	0.0	3.377	1.098	*
1	0	0	57.875	55.791	-55.791	0.0	2.080	0.657	*
1	0	0	94.038	95.617	-95.617	0.0	-2.584	-0.678	*
1	0	0	78.453	92.946	-92.946	0.0	-1.513	-0.513	*
1	0	0	27.799	83.266	-83.266	0.0	-2.507	-0.815	*
1	0	0	86.105	33.221	33.221	0.0	-5.022	-1.637	*
1	0	0	121.428	80.388	80.388	0.0	3.956	1.885	*
1	0	0	51.825	128.655	-128.655	0.0	-7.237	-2.360	*
1	0	0	45.525	55.756	-55.756	0.0	-3.258	-1.254	*
1	0	0	50.348	44.250	44.250	0.0	-1.175	-0.382	*
1	0	0	11.586	36.088	-36.088	0.0	8.588	2.912	*
1	0	0	37.240	4.721	-4.721	0.0	6.555	2.262	**
1	0	0	42.427	41.257	-41.257	0.0	-4.340	-1.476	*
1	0	0	20.450	43.852	-43.852	0.0	-4.951	-1.917	*
1	0	0	74.911	36.521	36.521	0.0	12.375	4.014	**
1	0	0	18.933	76.994	-76.994	0.0	-2.585	-0.832	**
1	0	0	93.485	16.385	16.385	0.0	-0.719	-0.299	**
1	0	0	53.341	79.059	-79.059	0.0	-2.729	-0.887	**
1	0	0	32.731	96.121	-96.121	0.0	11.359	3.804	*
1	0	0	44.744	21.082	21.082	0.0	-24.522	-7.844	*
1	0	0		348.182	-348.182	0.0	-0.590	-2.143	*
1	0	0		51.334	-51.334	0.0			

Table 2 (cont)
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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
-10	-4	0	74.353	74.438	-74.438	0.0	-0.085	-0.016
-12	-4	0	51.013	74.783	74.783	0.0	22.770	1.389
-14	-4	0	1.076	54.022	54.022	0.0	52.946	0.327
-16	-4	0	1.076	22.908	-22.908	0.0	-23.984	-3.010
-18	-4	0	128.041	48.748	-5.848	0.0	-3.081	-1.002
-20	-4	0	138.041	128.817	-126.817	0.0	-3.698	-1.202
-22	-4	0	23.176	35.925	48.748	0.0	1.258	0.409
-24	-4	0	5.826	28.738	-34.255	0.0	-1.756	-0.581
-26	-4	0	13.826	8.393	-54.393	0.0	-0.918	-0.299
-28	-4	0	17.741	18.423	-18.423	0.0	-0.167	-0.054
-30	-4	0	44.282	178.222	198.434	0.0	-6.108	-1.986
-32	-4	0	44.486	48.542	-48.222	0.0	-2.481	-0.807
-34	-4	0	19.874	64.672	64.672	0.0	4.800	1.385
-36	-4	0	40.870	20.522	-29.826	0.0	-0.150	-0.062
-38	-4	0	40.870	44.572	44.572	0.0	3.702	1.100
-40	-4	0	10.375	40.872	-40.872	0.0	-16.705	-5.415
-42	-4	0	20.752	106.199	106.199	0.0	85.827	4.844
-44	-4	0	54.123	20.790	-20.790	0.0	-0.551	-0.179
-46	-4	0	42.283	53.897	53.897	0.0	11.614	0.373
-48	-4	0	20.450	42.201	-42.201	0.0	-0.282	-0.027
-50	-4	0	3.240	14.021	14.021	0.0	11.049	2.097
-52	-4	0	1.638	29.572	29.572	0.0	28.934	2.494
-54	-4	0	56.454	36.149	-36.149	0.0	-20.305	-1.785
-56	-4	0	32.320	66.438	66.438	0.0	34.118	1.785
-58	-4	0	43.658	31.672	-31.672	0.0	-0.516	-0.005
-60	-4	0	38.470	47.735	47.735	0.0	9.267	0.211
-62	-4	0	18.820	41.610	41.610	0.0	22.790	1.313
-64	-4	0	8.572	16.769	-16.769	0.0	-8.197	-1.021
-66	-4	0	77.187	85.755	-85.755	0.0	-8.568	-0.667
-68	-4	0	20.235	76.706	-76.706	0.0	-54.471	-1.274
-70	-4	0	74.357	15.875	-15.875	0.0	-14.522	-0.156
-72	-4	0	34.811	58.045	58.045	0.0	23.234	1.418
-74	-4	0	79.278	75.251	-39.520	0.0	-14.759	-0.291
-76	-4	0	26.600	39.590	-73.420	0.0	-43.820	-1.554
-78	-4	0	1.741	25.685	-23.685	0.0	-21.944	-1.905
-80	-4	0	73.589	75.158	-21.722	0.0	-1.570	-0.297
-82	-4	0	44.129	15.859	-15.859	0.0	-14.538	-0.803
-84	-4	0	16.780	46.600	46.600	0.0	29.821	1.021
-86	-4	0	209.480	16.663	-16.663	0.0	-14.056	-0.521
-88	-4	0	56.823	211.186	211.186	0.0	154.363	5.555
-90	-4	0	132.478	71.189	-71.189	0.0	-61.289	-1.755
-92	-4	0	238.316	132.516	-132.516	0.0	-105.799	-3.012
-94	-4	0	44.067	63.109	-243.542	0.0	-289.475	-8.387
-96	-4	0	43.114	45.967	-45.967	0.0	-1.853	-0.068
-98	-4	0	138.847	40.435	-40.435	0.0	-98.412	-0.847
-100	-4	0	138.905	108.138	-108.138	0.0	-130.767	-0.745
-102	-4	0		141.085	-141.085	0.0	-2.180	-0.709

Table 2 (cont)
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H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/STGMA
-1	4	4	54.307	56.234	-56.234	0.0	-1.927	-0.627
-1	4	4	32.616	12.621	12.621	0.0	4.226	4.226
-1	4	4	38.636	36.784	36.784	0.0	0.042	0.042
-1	4	4	47.096	45.729	45.729	0.0	0.380	0.380
-1	4	4	77.777	75.703	-75.703	0.0	-0.548	-0.548
-1	4	4	53.310	51.892	51.892	0.0	-0.591	-0.591
-1	4	4	53.310	85.013	85.013	0.0	1.075	1.075
-1	4	4	114.707	8.322	-8.322	0.0	-3.135	-3.135
-1	4	4	147.175	114.427	114.427	0.0	0.840	0.840
-2	4	4	167.935	42.997	-42.997	0.0	0.058	0.058
-4	4	4	170.518	168.610	168.610	0.0	0.220	0.220
-4	4	4	97.907	164.807	164.807	0.0	1.857	1.857
-4	4	4	18.707	96.100	96.100	0.0	1.040	1.040
-6	4	4	17.897	11.335	11.335	0.0	-0.856	-0.856
-8	4	4	102.680	14.084	-14.084	0.0	1.240	1.240
-8	4	4	80.292	103.077	-103.077	0.0	-0.129	-0.129
-10	4	4	38.316	47.385	-47.385	0.0	-3.473	-3.473
-10	4	4	11.071	47.385	-47.385	0.0	-9.069	-9.069
-12	4	4	34.042	28.573	28.573	0.0	3.569	3.569
-12	4	4	75.649	74.551	74.551	0.0	1.097	1.097
-14	4	4	72.051	70.615	-70.615	0.0	0.357	0.357
-14	4	4	45.635	49.820	-49.820	0.0	0.466	0.466
-16	4	4	14.453	17.442	-17.442	0.0	-1.361	-1.361
-16	4	4	76.510	77.652	-77.652	0.0	-0.371	-0.371
-18	4	4	21.126	18.851	-18.851	0.0	0.740	0.740
-18	4	4	25.585	17.946	-17.946	0.0	2.478	2.478
-18	4	4	329.657	329.578	329.578	0.0	0.079	0.079
-18	4	4	132.724	128.826	-128.826	0.0	3.898	3.898
-20	4	4	15.161	96.308	-96.308	0.0	1.268	1.268
-20	4	4	96.068	96.537	-96.537	0.0	3.204	3.204
-20	4	4	52.062	57.754	-57.754	0.0	-0.152	-0.152
-20	4	4	29.399	33.585	-33.585	0.0	-1.851	-1.851
-20	4	4	42.529	36.836	-36.836	0.0	2.081	2.081
-20	4	4	42.529	42.436	-42.436	0.0	0.400	0.400
-20	4	4	36.840	36.450	-36.450	0.0	0.384	0.384
-20	4	4	201.700	196.832	-196.832	0.0	0.124	0.124
-20	4	4	175.038	173.335	-173.335	0.0	1.583	1.583
-20	4	4	141.519	127.394	-127.394	0.0	0.854	0.854
-20	4	4	47.327	39.832	-39.832	0.0	4.391	4.391
-20	4	4	32.381	36.694	-36.694	0.0	2.437	2.437
-20	4	4	96.714	90.219	-90.219	0.0	2.112	2.112
-20	4	4	78.078	83.133	-83.133	0.0	-0.584	-0.584
-20	4	4	76.264	75.337	-75.337	0.0	1.501	1.501
-20	4	4	41.668	37.821	-37.821	0.0	1.251	1.251
-20	4	4	53.692	55.192	-55.192	0.0	-0.183	-0.183
-20	4	4	76.326	69.827	-69.827	0.0	2.119	2.119
-20	4	4	174.849	170.761	-170.761	0.0	4.089	4.089
-20	4	4	113.873	114.090	-114.090	0.0	-0.217	-0.217
-20	4	4	50.002	45.475	-45.475	0.0	1.422	1.422
-20	4	4	28.089	83.058	-83.058	0.0	-1.182	-1.182
-20	4	4	28.291	29.410	-29.410	0.0	-0.364	-0.364

Table 2 (cont)
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HCLS 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
12	4	9	47.256	46.939	46.939	0.0	0.357	0.116	
14	4	9	57.509	57.509	57.509	0.0	-1.082	-0.352	
14	4	9	41.5043	41.5027	41.5027	0.0	4.116	1.338	*
14	4	9	16.624	16.5713	-16.5713	0.0	3.096	1.007	**
16	4	9	47.206	46.713	46.713	0.0	-3.513	-1.142	
18	4	9	49.787	47.523	47.523	0.0	6.194	2.014	*
18	4	9	96.007	93.628	93.628	0.0	2.378	0.773	**
18	4	9	118.101	117.219	117.219	0.0	3.882	1.262	*
18	4	9	199.301	194.528	-184.528	0.0	3.764	1.224	
18	4	9	40.008	30.658	-30.658	0.0	-1.357	-0.441	*
18	4	9	4.859	8.346	8.346	0.0	-3.487	-2.974	**
18	4	9	24.171	21.574	21.574	0.0	2.597	0.857	*
18	4	9	72.646	71.813	-71.813	0.0	0.834	0.278	
18	4	9	65.374	68.984	68.984	0.0	-1.617	-1.173	*
18	4	9	18.974	6.052	6.052	0.0	12.922	4.202	**
18	4	9	151.991	149.991	149.991	0.0	2.000	0.666	*
18	4	9	86.918	86.918	86.918	0.0	1.706	0.555	*
18	4	9	15.591	14.339	14.339	0.0	1.253	0.407	**
18	4	9	26.108	18.048	18.048	0.0	8.055	2.621	*
18	4	9	193.547	149.868	149.868	0.0	43.679	14.811	*
18	4	9	93.481	88.841	88.841	0.0	4.640	1.195	**
18	4	9	16.514	20.101	20.101	0.0	-3.586	-1.166	*
18	4	9	31.920	34.949	34.949	0.0	-3.029	-0.585	*
18	4	9	70.852	66.277	-66.277	0.0	4.573	1.510	*
18	4	9	138.659	140.277	140.277	0.0	-1.618	-0.526	*
18	4	9	39.208	31.551	31.551	0.0	7.657	2.490	*
18	4	9	87.888	88.750	-88.750	0.0	-0.862	-0.280	*
18	4	9	57.967	55.887	-55.887	0.0	2.070	0.676	**
18	4	9	3.567	15.166	15.166	0.0	-11.599	-3.572	*
18	4	9	52.432	44.708	-44.708	0.0	7.724	2.512	*
18	4	9	25.309	17.056	17.056	0.0	8.257	2.684	*
18	4	9	28.476	32.472	32.472	0.0	-4.006	-1.399	*
18	4	9	100.804	5.031	5.031	0.0	-4.047	-1.316	**
18	4	9	100.804	101.300	101.300	0.0	-0.496	-0.161	*
18	4	9	52.708	46.854	-46.854	0.0	5.854	1.804	*
18	4	9	11.593	0.790	-0.790	0.0	10.807	3.515	**
18	4	9	99.087	88.466	-88.466	0.0	10.621	3.202	*
18	4	9	17.471	120.603	120.603	0.0	-3.281	-1.012	*
18	4	9	94.284	92.003	-92.003	0.0	2.281	0.712	*
18	4	9	106.093	104.444	-104.444	0.0	1.649	0.536	*
18	4	9	8.426	0.736	0.736	0.0	7.690	2.563	**
18	4	9	60.704	52.514	-52.514	0.0	8.190	2.657	*
18	4	9	140.104	135.010	-135.010	0.0	5.094	1.657	*
18	4	9	40.900	39.772	-39.772	0.0	1.128	0.367	*
18	4	9	36.810	31.246	31.246	0.0	5.567	1.800	*
18	4	9	30.331	89.614	-89.614	0.0	3.717	1.209	*
18	4	9	100.436	99.303	-99.303	0.0	1.132	0.363	*
18	4	9	64.840	62.602	-62.602	0.0	2.238	0.663	*
18	4	9	22.725	24.220	24.220	0.0	-1.494	-0.484	**
18	4	9	87.427	92.267	-92.267	0.0	-4.840	-1.574	*
18	4	9	26.477	97.351	-97.351	0.0	-3.067	-1.097	*
18	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	52.171	48.068	48.068	0.0	3.103	1.009
-4	-4	10	74.773	74.210	74.210	0.0	0.563	-0.592
-6	-4	10	16.773	1.351	1.351	0.0	18.422	5.991
-8	-4	10	23.067	0.657	0.657	0.0	13.437	4.370
-8	-4	10	54.579	5.269	5.269	0.0	-11.048	-3.593
-10	-4	10	37.304	37.304	37.304	0.0	-11.048	-3.593
-12	-4	10	52.823	54.319	54.319	0.0	-1.496	-0.664
-12	-4	10	55.938	54.633	54.633	0.0	0.302	0.098
-15	-4	10	24.724	16.333	16.333	0.0	8.391	2.729
-15	-4	10	20.200	77.010	77.010	0.0	3.190	1.037
-15	-4	10	19.189	18.560	18.560	0.0	0.203	0.203
-15	-4	10	57.583	58.740	58.740	0.0	-1.158	-0.442
-17	-4	10	34.776	93.204	93.204	0.0	-1.573	-0.511
-17	-4	10	64.056	62.047	62.047	0.0	2.009	0.653
-19	-4	10	165.505	165.225	165.225	0.0	0.281	0.059
-19	-4	10	15.679	16.253	16.253	0.0	0.575	0.059
-21	-4	10	8.026	21.253	21.253	0.0	-13.227	-4.201
-21	-4	10	50.832	54.342	54.342	0.0	-3.510	-1.141
-22	-4	10	45.082	55.613	55.613	0.0	-10.531	-3.450
-22	-4	10	90.661	81.310	81.310	0.0	-9.349	-3.070
-24	-4	10	49.049	47.087	47.087	0.0	1.962	0.639
-24	-4	10	110.644	116.137	116.137	0.0	-5.493	-1.786
-28	-4	10	14.576	16.760	16.760	0.0	-2.184	-0.710
-28	-4	10	51.078	45.842	45.842	0.0	5.236	1.703
-30	-4	10	14.576	12.776	12.776	0.0	1.730	0.585
-32	-4	10	7.534	9.850	9.850	0.0	-2.323	-0.756
-34	-4	10	43.452	43.445	43.445	0.0	0.006	0.002
-34	-4	10	47.696	49.115	49.115	0.0	-1.419	-0.482
-35	-4	10	25.339	21.531	21.531	0.0	3.808	1.226
-35	-4	10	19.531	120.591	120.591	0.0	-1.775	-0.544
-35	-4	10	66.270	63.647	63.647	0.0	2.622	0.853
-35	-4	10	65.993	65.259	65.259	0.0	0.734	0.239
-35	-4	10	12.076	121.932	121.932	0.0	1.043	0.339
-37	-4	10	39.608	32.491	32.491	0.0	7.118	2.315
-38	-4	10	31.140	49.738	49.738	0.0	-1.402	-0.456
-38	-4	10	16.729	13.388	13.388	0.0	3.341	1.086
-38	-4	10	19.854	49.068	49.068	0.0	-3.214	-1.060
-38	-4	10	17.423	152.605	152.605	0.0	-5.182	-1.625
-40	-4	10	46.865	47.723	47.723	0.0	0.858	0.295
-40	-4	10	40.838	157.922	157.922	0.0	-10.087	-3.337
-41	-4	10	53.687	44.630	44.630	0.0	9.057	3.037
-41	-4	10	88.934	69.238	69.238	0.0	-18.692	-6.660
-41	-4	10	84.136	87.373	87.373	0.0	-3.237	-1.070
-41	-4	10	10.769	85.933	85.933	0.0	-1.561	-0.503
-42	-4	10	14.365	117.215	117.215	0.0	-11.043	-0.370
-42	-4	10	33.600	51.431	51.431	0.0	-17.831	-5.853
-42	-4	10	15.591	29.028	29.028	0.0	-13.437	-4.370
-42	-4	10	29.028	45.623	45.623	0.0	-16.643	-5.458
-44	-4	10	29.122	24.605	24.605	0.0	4.517	1.450

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	-0.082	-0.082	
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	-1.512	**
5	5	1	59.653	59.925	59.925	0.0	-0.272	-0.272	
5	5	1	22.616	20.192	20.192	0.0	2.424	2.424	
5	5	1	32.720	35.599	35.599	0.0	-2.879	-2.879	
5	5	1	44.559	52.960	52.960	0.0	-8.401	-8.401	*
5	5	1	15.530	13.347	13.347	0.0	2.183	2.183	**
5	5	1	100.250	100.058	100.058	0.0	0.192	0.192	
5	5	1	145.824	145.629	145.629	0.0	0.195	0.195	
5	5	1	73.958	71.874	71.874	0.0	2.084	2.084	
5	5	1	100.312	99.721	99.721	0.0	0.591	0.591	
5	5	1	97.322	99.826	99.826	0.0	-2.504	-2.504	
5	5	1	26.477	32.377	32.377	0.0	-5.900	-5.900	
5	5	1	61.472	66.359	66.359	0.0	-4.887	-4.887	
5	5	1	159.939	162.700	162.700	0.0	-2.761	-2.761	
5	5	1	35.949	37.983	37.983	0.0	-2.034	-2.034	
5	5	1	27.259	57.424	57.424	0.0	-30.165	-30.165	
5	5	1	44.436	40.741	40.741	0.0	3.695	3.695	
5	5	1	37.794	40.217	40.217	0.0	-2.423	-2.423	
5	5	1	16.729	21.785	21.785	0.0	-5.056	-5.056	*
5	5	1	59.837	77.237	77.237	0.0	-17.400	-17.400	**
5	5	1	130.602	123.086	123.086	0.0	7.516	7.516	
5	5	1	29.737	38.011	38.011	0.0	-8.274	-8.274	
5	5	1	61.134	60.735	60.735	0.0	0.399	0.399	
5	5	1	15.830	137.026	137.026	0.0	-121.196	-121.196	
5	5	1	18.605	10.091	10.091	0.0	8.514	8.514	
5	5	1	106.862	106.585	106.585	0.0	0.277	0.277	
5	5	1	69.437	74.186	74.186	0.0	-4.748	-4.748	
5	5	1	12.977	12.743	12.743	0.0	0.234	0.234	*
5	5	1	20.942	13.869	13.869	0.0	7.073	7.073	**
5	5	1	8.974	10.705	10.705	0.0	-2.033	-2.033	*
5	5	1	45.974	43.708	43.708	0.0	2.265	2.265	**
5	5	1	88.026	89.594	89.594	0.0	-1.568	-1.568	
5	5	1	39.454	37.945	37.945	0.0	1.509	1.509	
5	5	1	76.326	77.608	77.608	0.0	-1.282	-1.282	
5	5	1	87.304	84.767	84.767	0.0	2.537	2.537	
5	5	1	32.396	38.332	38.332	0.0	-5.936	-5.936	
5	5	1	32.443	27.857	27.857	0.0	4.586	4.586	
5	5	1	87.058	88.105	88.105	0.0	-1.047	-1.047	
5	5	1	187.093	187.871	187.871	0.0	-0.778	-0.778	
5	5	1	26.761	69.154	69.154	0.0	-42.393	-42.393	
5	5	1	100.329	99.984	99.984	0.0	0.345	0.345	
5	5	1	18.153	105.928	105.928	0.0	-2.225	-2.225	
5	5	1	16.468	17.468	17.468	0.0	-1.000	-1.000	*
5	5	1	42.929	153.801	153.801	0.0	-110.872	-110.872	**
5	5	1	59.441	59.441	59.441	0.0	0.000	0.000	
5	5	1				0.0	3.489	3.489	

Table 2 (cont)
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HCLB 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
1	5	4	19.404	11.414	11.414	0.0	7.990	2.598
1	5	4	49.329	50.359	-28.379	0.0	-1.030	-0.534
1	5	4	40.654	42.837	-42.834	0.0	-2.183	-1.762
1	5	4	49.125	73.801	-73.801	0.0	-3.704	-0.051
1	5	4	83.757	76.660	-76.660	0.0	-3.108	2.308
1	5	4	35.303	38.800	-38.800	0.0	-3.497	-1.137
1	5	4	124.300	124.567	124.567	0.0	0.267	-0.067
1	5	4	8.426	6.388	32.038	0.0	2.612	0.663
1	5	4	39.700	48.431	-48.431	0.0	-8.731	2.241
1	5	4	50.525	22.319	-22.319	0.0	-2.094	0.681
1	5	4	26.508	28.890	-28.890	0.0	-4.189	0.125
1	5	4	29.276	24.830	-24.830	0.0	-4.446	0.125
1	5	4	8.610	36.830	-36.830	0.0	-3.720	0.426
1	5	4	23.525	23.752	-23.752	0.0	-0.227	0.496
1	5	4	20.296	18.770	-18.770	0.0	-1.474	0.496
1	5	4	21.527	17.696	-17.696	0.0	-3.831	2.327
1	5	4	14.177	134.177	-134.177	0.0	-120.000	0.884
1	5	4	14.064	16.804	-16.804	0.0	-2.740	0.772
1	5	4	20.644	12.109	-12.109	0.0	-8.535	0.246
1	5	4	27.154	26.448	-26.448	0.0	-0.706	0.007
1	5	4	45.411	45.471	-45.471	0.0	-0.060	0.187
1	5	4	103.500	99.859	-99.859	0.0	-3.641	0.687
1	5	4	24.099	21.955	-21.955	0.0	-2.144	0.616
1	5	4	17.098	18.992	-18.992	0.0	-1.894	0.401
1	5	4	91.092	79.857	-79.857	0.0	-1.235	0.401
1	5	4	33.222	24.703	-24.703	0.0	-8.519	2.797
1	5	4	25.801	25.690	-25.690	0.0	-0.110	0.036
1	5	4	93.811	60.334	-60.334	0.0	-3.477	0.150
1	5	4	36.041	35.816	-35.816	0.0	-0.225	0.065
1	5	4	60.450	60.802	-60.802	0.0	-0.352	0.072
1	5	4	79.493	77.073	-77.073	0.0	-2.420	0.182
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	15.329	6.966	-6.966	0.0	-8.363	0.915
1	5	4	27.584	24.827	-24.827	0.0	-2.757	1.093
1	5	4	70.975	64.852	-64.852	0.0	-6.123	0.491
1	5	4	21.417	42.416	-42.416	0.0	-21.000	0.651
1	5	4	18.205	17.501	-17.501	0.0	-0.704	0.229
1	5	4	29.508	26.507	-26.507	0.0	-3.001	0.000
1	5	4	47.450	40.591	-40.591	0.0	-6.859	2.230
1	5	4	31.372	9.844	-9.844	0.0	-2.512	0.817
1	5	4	47.444	5.225	-5.225	0.0	-42.217	0.310
1	5	4	17.702	196.023	-196.023	0.0	-178.321	0.416
1	5	4	32.714	74.333	-74.333	0.0	-41.619	0.302
1	5	4	37.911	37.911	0.0	0.0	0.000	0.265
1	5	4	98.451	97.436	-97.436	0.0	-1.015	0.015

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	0.00	8.106	2.636	
-1	5	8	132.249	27.070	-27.070	0.00	-13.477	-4.383	**
-1	5	8	49.848	100.635	-100.635	0.00	1.621	0.525	**
-1	5	8	59.222	46.028	76.028	0.00	-6.803	1.242	
0	5	9	40.158	41.800	-33.800	0.00	4.358	1.417	
0	5	9	35.518	20.262	-33.800	0.00	1.570	0.511	**
0	5	9	129.737	16.725	-19.725	0.00	10.012	-2.179	**
0	5	9	129.099	120.131	-36.480	0.00	3.374	0.965	
0	5	9	44.213	45.004	45.004	0.00	-0.691	1.097	
0	5	9	22.449	28.713	28.713	0.00	11.698	0.157	
0	5	9	40.039	10.751	-33.687	0.00	6.332	2.804	
0	5	9	139.198	138.908	138.908	0.00	-0.231	2.066	
0	5	9	50.617	54.145	-54.145	0.00	-0.711	1.147	
0	5	9	50.365	41.225	-41.225	0.00	-3.356	0.714	
0	5	9	76.141	62.744	62.744	0.00	-3.179	1.034	
0	5	9	41.576	45.259	-45.259	0.00	-3.893	1.198	
0	5	9	38.954	83.901	83.901	0.00	18.007	1.647	**
0	5	9	20.019	1.708	1.708	0.00	18.007	3.954	**
0	5	9	14.322	19.900	19.900	0.00	5.470	1.798	**
0	5	9	134.063	30.033	-30.033	0.00	12.510	1.766	**
0	5	9	132.852	128.255	-128.255	0.00	4.702	1.403	**
0	5	9	31.920	29.899	-29.899	0.00	7.316	1.302	**
0	5	9	46.927	24.005	24.005	0.00	-5.914	2.574	**
0	5	9	22.110	20.007	-20.007	0.00	-1.707	1.737	**
0	5	9	13.930	18.516	-18.516	0.00	-14.054	0.684	**
0	5	9	18.651	17.884	-17.884	0.00	0.305	4.570	**
0	5	9	54.701	57.810	-57.810	0.00	6.802	0.929	**
0	5	9	27.779	23.779	-23.779	0.00	-3.008	2.241	**
0	5	9	70.505	10.952	-10.952	0.00	4.442	0.002	**
0	5	9	9.035	26.064	26.064	0.00	1.121	1.121	**
0	5	9	58.091	80.081	80.081	0.00	0.988	0.321	**
0	5	9	16.218	29.353	29.353	0.00	-1.323	4.958	**
0	5	9	107.093	103.893	-103.893	0.00	1.096	0.320	**
0	5	9	179.005	31.070	-31.070	0.00	-13.235	1.321	**
0	5	9	14.004	15.997	-15.997	0.00	-1.096	0.320	**
0	5	9	11.004	16.014	-16.014	0.00	-10.512	0.320	**
0	5	9	45.007	49.184	-49.184	0.00	-3.210	0.145	**
0	5	9	33.033	74.588	74.588	0.00	1.044	0.708	**
0	5	9	11.258	93.588	93.588	0.00	-3.454	1.854	**
0	5	9	11.258	18.529	-18.529	0.00	1.580	1.854	**
0	5	9	77.771	76.618	-76.618	0.00	-1.153	0.320	**
0	5	9	124.000	103.132	-103.132	0.00	-2.082	0.320	**
0	5	9	17.000	20.512	-20.512	0.00	-5.972	0.145	**
0	5	9	8.150	74.769	-74.769	0.00	-1.203	1.203	**
0	5	9	8.150	20.653	-20.653	0.00	-12.473	-4.056	**

Table 2 (cont)
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H	K	L	F (OBS)	F (CALC)	A (CALC)	B (CALC)	DELTA F	DELTA F / SIGMA
-14	0	0	62.672	60.532	-60.532	0.000	2.140	0.696
-11	0	0	37.972	36.441	40.441	0.000	-4.469	-0.801
13	0	0	85.028	84.892	89.892	0.000	-4.864	-1.582
5	0	0	13.254	14.870	-24.870	0.000	-2.770	-0.907
5	0	0	69.275	77.203	14.203	0.000	-0.909	-0.309
5	0	0	26.754	12.122	-12.122	0.000	7.770	2.523
7	0	0	11.860	17.521	-17.521	0.000	4.683	1.255
0	0	0	23.709	82.261	-82.261	0.000	-2.709	-0.881
0	0	0	160.001	153.381	153.381	0.000	-5.960	-1.821
1	0	0	180.775	180.972	-80.972	0.000	3.447	1.121
1	0	0	44.774	42.652	-42.652	0.000	1.853	0.603
1	0	0	15.944	72.372	-72.372	0.000	9.473	3.168
1	0	0	71.251	37.700	-72.372	0.000	1.244	0.366
1	0	0	42.724	35.876	-25.876	0.000	5.229	1.700
1	0	0	15.038	11.816	-11.816	0.000	1.112	0.362
2	0	0	97.636	98.058	-98.058	0.000	3.421	1.113
2	0	0	38.962	40.050	-40.050	0.000	-0.432	-0.140
2	0	0	18.389	23.029	-23.029	0.000	1.537	0.539
4	0	0	41.453	44.007	-44.007	0.000	4.056	1.517
4	0	0	109.322	104.007	104.007	0.000	-2.570	-0.836
6	0	0	85.151	83.069	-83.069	0.000	2.255	1.406
6	0	0	17.733	19.370	-19.370	0.000	1.643	0.697
8	0	0	114.622	114.622	114.622	0.000	-0.529	-0.179
10	0	0	157.659	160.611	-160.611	0.000	1.550	0.960
10	0	0	115.780	113.174	113.174	0.000	-2.498	-0.847
11	0	0	26.231	24.710	-24.710	0.000	1.512	0.492
11	0	0	47.850	46.919	-46.919	0.000	0.930	0.303
11	0	0	24.847	9.785	-9.785	0.000	15.063	4.898
14	0	0	50.555	50.710	-50.710	0.000	-0.155	-0.050
14	0	0	41.299	40.312	-40.312	0.000	0.986	0.311
15	0	0	75.865	55.961	-55.961	0.000	0.956	0.311
15	0	0	71.133	71.133	-71.133	0.000	0.000	0.000
15	0	0	80.588	84.610	-84.610	0.000	4.022	1.549
17	0	0	19.158	12.312	-12.312	0.000	6.846	2.224
17	0	0	21.598	36.112	-36.112	0.000	1.664	0.520
19	0	0	46.988	43.675	-43.675	0.000	3.313	1.077
19	0	0	92.310	90.147	-90.147	0.000	2.163	0.735
19	0	0	16.310	28.248	-28.248	0.000	11.924	3.866
19	0	0	35.344	40.558	-40.558	0.000	5.214	1.699
19	0	0	16.520	30.749	-30.749	0.000	14.224	4.619
19	0	0	12.218	12.218	-12.218	0.000	0.000	0.000
19	0	0	64.882	64.882	-64.882	0.000	0.000	0.000
19	0	0	3.842	3.842	-3.842	0.000	0.000	0.000
19	0	0	4.331	4.331	-4.331	0.000	0.000	0.000
19	0	0	15.520	97.890	-97.890	0.000	11.806	3.642
19	0	0	95.084	69.825	-69.825	0.000	2.264	0.713
4	0	0	66.577	68.600	-68.600	0.000	-2.023	-0.612
4	0	0	70.483	63.170	-63.170	0.000	7.313	2.402
4	0	0	56.706	61.102	-61.102	0.000	4.583	1.492
4	0	0	11.679	11.679	-11.679	0.000	0.000	0.000
8	0	0	83.675	83.740	-83.740	0.000	-0.065	-0.021

Table 2 (cont)
PAGE 25

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA F / SIGMA	STRUCTURE FACTORS
10	0	4	115.642	114.943	114.943	0.0	0.039	0.032	
10	0	4	55.071	55.459	-65.970	0.0	-0.388	-0.116	
11	0	4	30.717	40.970	-43.970	0.0	14.002	4.553	
11	0	4	13.717	43.134	-140.210	0.0	-4.073	-1.324	
11	0	5	17.903	140.210	111.297	0.0	5.163	2.828	
11	0	5	37.671	52.742	-42.099	0.0	-5.163	-1.679	
11	0	5	18.087	42.099	87.697	0.0	1.390	0.452	
11	0	5	105.764	100.599	-100.599	0.0	1.773	0.577	
11	0	5	57.414	57.135	-27.405	0.0	8.359	2.718	
11	0	5	57.135	77.135	-77.135	0.0	2.279	0.741	*
11	0	5	64.512	64.512	-13.310	0.0	2.866	0.932	**
11	0	5	55.377	55.377	-55.312	0.0	0.864	0.281	
11	0	5	60.012	60.012	-40.994	0.0	3.725	0.886	
11	0	5	46.250	44.323	80.429	0.0	3.717	1.079	
11	0	5	93.278	80.441	78.429	0.0	1.888	0.614	
11	0	5	75.580	78.441	-58.471	0.0	2.823	0.925	
11	0	5	32.950	58.639	10.712	0.0	-3.941	-1.048	*
11	0	5	17.060	10.712	-10.712	0.0	7.273	2.365	**
11	0	5	45.666	49.102	49.102	0.0	-3.436	-1.117	
11	0	5	27.000	30.776	30.776	0.0	-0.770	-0.226	
11	0	5	44.528	44.747	-44.747	0.0	0.219	0.071	
11	0	5	77.559	72.844	-72.844	0.0	4.711	1.532	
11	0	5	67.105	80.999	-80.999	0.0	-5.106	-1.600	*
11	0	5	17.657	11.411	-11.411	0.0	6.244	1.921	**
11	0	7	154.971	154.971	-154.971	0.0	4.346	1.271	*
11	0	7	20.877	17.445	-20.877	0.0	17.445	5.116	**
11	0	7	17.905	20.814	-20.814	0.0	3.911	1.111	*
11	0	7	38.691	93.789	93.789	0.0	7.979	2.582	
11	0	7	43.913	48.605	48.605	0.0	0.691	0.101	
11	0	7	11.563	10.946	-10.946	0.0	0.614	0.200	*
11	0	7	44.159	45.873	-45.873	0.0	-1.714	-0.557	**
11	0	7	94.715	99.471	99.471	0.0	-4.756	-1.546	
11	0	7	42.960	39.755	39.755	0.0	3.204	1.042	*
11	0	7	20.850	9.114	-9.114	0.0	11.735	3.816	
11	0	7	45.420	40.725	40.725	0.0	-4.695	-1.482	*
11	0	8	19.174	9.390	9.390	0.0	9.784	3.057	**
11	0	8	101.511	102.949	-102.949	0.0	-1.438	-0.466	*
11	0	8	8.703	1.158	-1.158	0.0	7.545	2.433	**
11	0	8	45.512	25.286	-25.286	0.0	-7.173	-2.373	**
11	0	8	54.031	46.949	-46.949	0.0	-11.436	-3.727	**
11	0	8	25.821	55.795	-55.795	0.0	-1.765	-0.547	*
11	0	8	93.971	27.190	-27.190	0.0	4.277	1.391	*
11	0	8	17.259	89.700	-89.700	0.0	-2.072	-0.671	*
11	0	8	97.175	173.328	173.328	0.0	0.531	0.173	*
11	0	8	67.008	96.644	-96.644	0.0	-3.871	-1.259	*
11	0	8	26.010	70.879	70.879	0.0	13.871	4.260	*
11	0	8	27.069	22.910	-22.910	0.0	-4.295	-1.397	*
11	0	8	21.649	32.070	32.070	0.0	-10.421	-3.359	**

Table 2 (cont)
PAGE#26

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)	DELTA F	DELTA/SIGMA
1	0	0	53.706	53.845	53.845	0.0	2.961	0.930
1	0	0	49.450	49.450	49.450	0.0	0.859	0.466
1	0	0	31.624	31.624	31.624	0.0	1.034	0.455
1	0	0	53.256	53.256	53.256	0.0	-0.502	-0.502
1	0	0	27.994	27.994	27.994	0.0	-1.562	-1.562
1	0	0	56.189	56.189	56.189	0.0	-0.056	-0.056
1	0	0	37.789	37.789	37.789	0.0	-0.324	-0.324
1	0	0	62.255	62.255	62.255	0.0	0.380	0.380
1	0	0	10.485	10.485	10.485	0.0	0.210	0.210
1	0	0	73.129	73.129	73.129	0.0	0.565	0.565
1	0	0	42.526	42.526	42.526	0.0	-0.187	-0.187
1	0	0	47.344	47.344	47.344	0.0	0.061	0.061
1	0	0	7.101	7.101	7.101	0.0	0.182	0.182
1	0	0	12.053	12.053	12.053	0.0	-0.394	-0.394
1	0	0	40.729	40.729	40.729	0.0	-2.163	-2.163
1	0	0	75.907	75.907	75.907	0.0	9.532	9.532
1	0	0	18.790	18.790	18.790	0.0	-2.649	-2.649
1	0	0	72.249	72.249	72.249	0.0	6.461	6.461
1	0	0	18.508	18.508	18.508	0.0	-4.812	-4.812
1	0	0	11.923	11.923	11.923	0.0	-0.727	-0.727
1	0	0	35.244	35.244	35.244	0.0	7.742	7.742
1	0	0	56.250	56.250	56.250	0.0	2.218	2.218
1	0	0	20.589	20.589	20.589	0.0	-1.390	-1.390
1	0	0	16.899	16.899	16.899	0.0	-3.327	-3.327
1	0	0	43.945	43.945	43.945	0.0	9.374	9.374
1	0	0	45.415	45.415	45.415	0.0	8.686	8.686
1	0	0	16.665	16.665	16.665	0.0	0.183	0.183
1	0	0	99.897	99.897	99.897	0.0	2.531	2.531
1	0	0	77.924	77.924	77.924	0.0	7.752	7.752
1	0	0	30.987	30.987	30.987	0.0	1.869	1.869
1	0	0	36.811	36.811	36.811	0.0	-2.849	-2.849
1	0	0	21.770	21.770	21.770	0.0	4.627	4.627
1	0	0	22.283	22.283	22.283	0.0	1.471	1.471
1	0	0	82.370	82.370	82.370	0.0	2.421	2.421
1	0	0	105.040	105.040	105.040	0.0	-0.452	-0.452
1	0	0	66.863	66.863	66.863	0.0	-1.448	-1.448
1	0	0	24.885	24.885	24.885	0.0	0.007	0.007
1	0	0	118.774	118.774	118.774	0.0	-0.576	-0.576
1	0	0	53.137	53.137	53.137	0.0	-3.058	-3.058
1	0	0	69.082	69.082	69.082	0.0	1.059	1.059
1	0	0	33.890	33.890	33.890	0.0	-0.540	-0.540
1	0	0	76.396	76.396	76.396	0.0	-3.453	-3.453
1	0	0	22.581	22.581	22.581	0.0	2.681	2.681
1	0	0	8.589	8.589	8.589	0.0	4.047	4.047
1	0	0	76.343	76.343	76.343	0.0	1.705	1.705
1	0	0	41.693	41.693	41.693	0.0	0.524	0.524
1	0	0	76.361	76.361	76.361	0.0	-6.343	-6.343
1	0	0	1.616	1.616	1.616	0.0	-0.112	-0.112
1	0	0	106.403	106.403	106.403	0.0	8.315	8.315
1	0	0	36.337	36.337	36.337	0.0	-0.370	-0.370
1	0	0	24.823	24.823	24.823	0.0	1.584	1.584
1	0	0	24.823	24.823	24.823	0.0	7.021	7.021

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	*
1	7	4	61.534	57.569	-57.569	0.0	3.965	1.289	
1	7	4	102.987	101.581	-101.581	0.0	1.407	0.457	
1	7	4	72.5279	70.429	-70.429	0.0	-0.685	-0.685	
1	7	4	133.282	129.524	-129.524	0.0	0.044	0.044	
1	7	4	131.861	129.524	-129.524	0.0	1.758	0.572	
1	7	4	90.231	85.565	-85.565	0.0	-0.798	-0.798	
1	7	5	43.725	42.562	-42.562	0.0	0.758	0.758	
1	7	5	87.738	80.921	-80.921	0.0	0.341	0.341	
1	7	5	58.121	56.900	-56.900	0.0	1.167	1.167	
1	7	5	53.765	50.399	-50.399	0.0	0.596	0.596	
1	7	5	53.275	52.139	-52.139	0.0	1.265	1.265	
1	7	5	43.567	43.742	-43.742	0.0	0.530	0.530	
1	7	5	31.244	34.305	-34.305	0.0	-0.349	-0.349	
1	7	5	37.886	41.323	-41.323	0.0	-0.075	-0.075	
1	7	5	19.820	24.925	-24.925	0.0	-3.961	-0.996	
1	7	5	145.886	100.600	-100.600	0.0	5.155	1.095	*
1	7	5	32.602	145.079	-145.079	0.0	3.740	1.216	**
1	7	5	130.049	12.016	-12.016	0.0	0.849	0.276	
1	7	5	43.698	32.812	-32.812	0.0	10.524	3.422	
1	7	7	55.378	61.471	-61.471	0.0	10.886	3.540	
1	7	7	39.270	43.456	-43.456	0.0	-4.226	-1.374	*
1	7	7	22.387	26.426	-26.426	0.0	-4.039	-1.313	**
1	7	7	31.059	30.129	-30.129	0.0	0.730	0.302	*
1	7	8	18.528	27.390	-27.390	0.0	-0.708	-0.844	**
1	7	8	44.857	59.931	-59.931	0.0	1.473	0.512	*
1	7	8	48.618	40.444	-40.444	0.0	1.705	0.585	
1	7	8	70.144	79.955	-79.955	0.0	-0.811	-3.190	**
1	7	8	13.598	20.718	-20.718	0.0	0.577	2.007	*
1	7	8	39.197	117.311	-117.311	0.0	-0.687	-2.139	**
1	7	8	56.214	63.162	-63.162	0.0	-3.665	-2.580	*
1	7	8	140.227	17.957	-17.957	0.0	1.785	0.580	**
1	7	8	19.588	142.012	-142.012	0.0	-5.697	-1.289	*
1	7	8	19.476	13.861	-13.861	0.0	1.552	0.580	**
1	7	8	53.324	107.923	-107.923	0.0	-2.527	-0.522	*
1	7	8	35.344	52.857	-52.857	0.0	1.527	0.522	*
1	7	8	15.235	55.881	-55.881	0.0	-3.346	-0.822	*
1	7	8	15.235	32.019	-32.019	0.0	1.503	4.786	*
1	7	8	15.235	14.588	-14.588	0.0	-2.690	-0.819	*
1	7	8	15.235	105.933	-105.933	0.0	-4.696	-0.819	*
1	7	8	15.235	161.954	-161.954	0.0	-7.637	-2.483	*
1	7	8	15.235	13.366	-13.366	0.0	1.576	0.576	*
1	7	8	15.235	114.050	-114.050	0.0	-2.269	-2.344	**
1	7	8	15.235	74.039	-74.039	0.0	2.687	0.874	*

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	
2	-8	4	37.056	19.328	19.328	0.0	17.728	5.765	
0	-8	4	32.566	28.830	28.830	0.0	3.736	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 ₂ 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 ₂ 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 ₂ 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 ₂ 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(13)
H ₂ 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 ₂ 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 ₂ 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 ± 0.005 Å, etc.

End of supplemental material.