

## The crystal structure of santaclaraite,<sup>1</sup> $\text{CaMn}_4[\text{Si}_5\text{O}_{14}(\text{OH})](\text{OH})\cdot\text{H}_2\text{O}$ : the role of hydrogen atoms in the pyroxenoid structure

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### Abstract

A new mineral, santaclaraite ( $\text{Ca}_{0.90}\text{Mn}_{4.04}\text{Mg}_{0.05}\text{Fe}_{0.01}^{2+}[\text{Si}_5\text{O}_{14}(\text{OH})](\text{OH})\cdot\text{H}_2\text{O}$ ), is triclinic with  $a = 10.273(4)$ ,  $b = 11.910(4)$ ,  $c = 12.001(6)\text{\AA}$ ,  $\alpha = 105.77(3)$ ,  $\beta = 110.64(3)$ ,  $\gamma = 87.13(3)^\circ$ ,  $V = 1317.0(8)\text{\AA}^3$ ;  $Z = 4$  for the  $\bar{1}$  unit-cell setting. The crystal structure consists of alternating tetrahedral and octahedral layers. The tetrahedral layer is made up of infinite single chains of silicate tetrahedra with a repeat period of five tetrahedra. The octahedral layer includes rows of ten octahedra with adjacent octahedral rows displaced along their length to form bands two or three octahedra wide. As isolated units, the tetrahedral chain and octahedral band of santaclaraite are similar to the corresponding portions of the rhodonite structure. The structure of santaclaraite, however, differs in that (1) two adjacent chains (or bands) in a given layer are displaced by a half  $c$  translation, and (2) the octahedral layer is rotated by a half turn in the plane parallel to the layer with respect to the adjacent tetrahedral layer. The three roles of hydrogen as hydrogen bond, hydroxyl group, and water molecule are responsible for the above half-translation and half-rotation. Three octahedral sites, M1, M2, and M3, are essentially occupied by Mn atoms. The Ca atoms are ordered in M5, and the small amount of Mg is probably concentrated in M4. Differential thermal analysis and thermogravimetric analysis indicate that the dehydration of santaclaraite occurs at approximately  $550^\circ\text{C}$ .

### Introduction

Santaclaraite, a new mineral from the Franciscan formation, Santa Clara County, California, is structurally related to rhodonite, babingtonite, nambulite, and marsturite (Ohashi and Erd, 1978). The mineral description is given elsewhere (Erd and Ohashi, in preparation). Santaclaraite is chemically equivalent to rhodonite plus two water molecules,  $\text{CaMn}_4\text{Si}_5\text{O}_{15}$  (rhodonite) +  $2\text{H}_2\text{O}$ ; its water content is less than that of inesite,  $\text{CaMn}_3[\text{Si}_5\text{O}_{14}(\text{OH})]\cdot 2.5\text{H}_2\text{O}$ , but more than that of babingtonite,  $\text{Ca}_2(\text{Fe},\text{Mn})\text{Fe}^{2+}[\text{Si}_5\text{O}_{14}(\text{OH})]$ , nambulite,  $(\text{Li},\text{Na})\text{Mn}_4[\text{Si}_5\text{O}_{14}(\text{OH})]$ , and marsturite,  $\text{NaCaMn}_3[\text{Si}_5\text{O}_{14}(\text{OH})]$ , another recently discovered pyroxenoid (Peacor *et al.*, 1978a).

The importance of octahedral cations in controlling the octahedral-tetrahedral linkages in the pyroxenoid structure has previously been discussed for three-tetrahedral-repeat pyroxenoids (Ohashi and Finger, 1978). The octahedral cations are identical in rhodonite and santaclaraite, so the different structures must be due to effects produced by the hydrogen atoms.

Inesite, a double-chain silicate with a five-tetrahedral repeat, has two crystal-chemically distinct types of hydrogen atoms, one as  $\text{H}_2\text{O}$  and the other as  $\text{OH}^-$  (Wan and Ghose, 1975, 1978). The hydrogen in babingtonite (Araki and Zoltai, 1972) and nambulite (Narita *et al.*, 1975; Murakami *et al.*, 1977) is believed to form a hydrogen bond  $\text{O}-\text{H}\cdots\text{O}$ , on the basis of the short  $\text{O}-\text{O}$  distance, as in pectolite (Prewitt and Buerger, 1963; Takéuchi and Kudoh, 1978).

Santaclaraite is unique among pyroxenoid miner-

<sup>1</sup> Approved by the Commission on New Minerals and Mineral Names, IMA.

(Contact/Parasite Structure Factor Table (based on H-cell))

H	K	L	F(CBS)	F(CALC)	H	K	L	F(CBS)	F(CALC)
-17	0	1	22.850	17.089	21	0	3	16.874	15.777
-15	0	1	26.138	23.784	-20	0	4	34.146	33.263
-13	0	1	17.943	14.986	-18	0	4	14.780	10.337
-11	0	1	39.959	39.278	-16	0	4	12.463	16.467
-9	0	1	58.963	53.117	-14	0	4	37.508	37.633
-7	0	1	73.724	68.132	-12	0	4	55.630	52.666
-5	0	1	174.492	163.450	-10	0	4	79.992	76.784
-1	0	1	45.919	48.255	-8	0	4	95.476	91.876
1	0	1	5.703	8.950	-6	0	4	34.598	36.778
3	0	1	35.988	32.911	-2	0	4	27.748	28.725
5	0	1	27.089	28.550	0	0	4	50.171	48.750
7	0	1	222.228	214.926	2	0	4	89.053	90.708
9	0	1	411.000	411.353	4	0	4	340.675	334.182
11	0	1	17.528	36.206	6	0	4	73.236	69.457
13	0	1	104.492	101.368	8	0	4	183.411	181.084
15	0	1	37.195	35.897	10	0	4	45.317	44.119
17	0	1	21.659	18.694	12	0	4	125.045	120.530
19	0	1	15.224	14.427	14	0	4	56.049	53.932
-20	0	2	36.837	34.613	16	0	4	12.577	12.925
-18	0	2	71.797	68.542	18	0	4	54.224	50.805
-16	0	2	30.626	25.736	20	0	4	18.228	14.173
-14	0	2	110.626	106.888	-19	0	5	62.089	58.149
-12	0	2	88.138	83.666	-17	0	5	170.825	163.394
-10	0	2	122.841	122.792	-15	0	5	176.183	170.654
-8	0	2	104.675	104.102	-13	0	5	42.719	40.234
-6	0	2	21.313	23.721	-11	0	5	58.171	60.144
-4	0	2	53.915	49.589	-9	0	5	50.659	50.199
-2	0	2	24.260	21.488	-7	0	5	40.106	22.372
0	0	2	31.659	31.296	-5	0	5	36.061	52.318
2	0	2	27.813	17.279	-3	0	5	66.496	61.552
4	0	2	163.967	156.700	-1	0	5	30.305	23.934
6	0	2	69.740	68.928	1	0	5	55.411	52.899
8	0	2	123.886	126.489	3	0	5	168.073	168.434
14	0	2	107.553	105.739	5	0	5	22.057	26.301
16	0	2	126.687	120.793	7	0	5	18.451	19.722
18	0	2	78.488	77.213	9	0	5	22.406	24.482
-19	0	3	21.984	16.835	11	0	5	56.768	53.293
-17	0	3	42.756	41.647	13	0	5	249.606	241.392
-15	0	3	23.573	23.978	15	0	5	16.890	20.620
-13	0	3	11.268	12.557	17	0	5	85.813	83.767
-11	0	3	27.264	29.163	19	0	5	40.207	39.496
-9	0	3	76.370	77.803	-20	0	6	23.309	19.236
-7	0	3	60.785	58.575	-18	0	6	33.967	34.661
-5	0	3	126.065	129.039	-16	0	6	88.187	83.976
-3	0	3	17.606	11.769	-14	0	6	38.976	37.470
-1	0	3	76.028	69.386	-10	0	6	116.732	111.260
1	0	3	55.419	58.142	-8	0	6	237.675	224.662
3	0	3	64.740	65.131	-6	0	6	245.325	238.424
5	0	3	74.748	71.991	-4	0	6	116.386	111.831
7	0	3	58.280	57.786	-2	0	6	88.797	88.388
9	0	3	17.740	16.402	0	0	6	146.390	140.006
13	0	3	27.874	33.834	2	0	6	20.776	18.127
17	0	3	81.776	85.135	4	0	6	74.333	70.674

Gantaciarite Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
8	0	6	26.553	35.814	-14	0	10	42.240	44.023
0	0	6	105.248	101.626	-12	0	10	32.037	29.937
2	0	6	152.573	151.609	-8	0	10	54.406	50.412
4	0	6	33.167	33.129	-6	0	10	29.354	26.921
8	0	6	24.589	27.632	-4	0	10	199.179	198.528
9	0	7	15.224	11.896	-2	0	10	152.163	151.019
5	0	7	28.817	24.409	0	0	10	17.297	16.406
3	0	7	13.122	11.810	2	0	10	30.362	31.779
1	0	7	74.715	71.261	4	0	10	90.557	87.543
9	0	7	20.146	11.828	6	0	10	25.711	22.481
5	0	7	68.504	67.399	8	0	10	27.805	30.425
3	0	7	36.049	37.490	14	0	10	67.236	63.828
1	0	7	232.972	224.119	16	0	10	19.504	21.290
1	0	7	150.094	145.854	-15	0	11	14.890	2.010
3	0	7	120.150	119.943	-9	0	11	68.163	66.190
5	0	7	42.793	40.363	-7	0	11	79.102	79.717
7	0	7	97.614	91.948	-5	0	11	104.768	104.564
9	0	7	67.175	64.297	-3	0	11	51.390	52.293
1	0	7	63.159	65.280	-1	0	11	20.467	20.124
3	0	7	53.520	50.719	1	0	11	13.854	16.162
5	0	7	67.443	65.419	3	0	11	115.858	113.327
7	0	7	13.541	16.009	5	0	11	161.285	161.240
9	0	7	52.516	51.074	7	0	11	82.630	81.064
0	0	8	46.163	43.914	9	0	11	52.411	52.417
3	0	8	26.549	23.978	11	0	11	37.394	37.146
5	0	8	38.785	34.655	13	0	11	65.915	66.723
7	0	8	94.906	91.471	-14	0	12	36.691	34.532
9	0	8	53.171	51.267	-12	0	12	14.179	12.266
0	0	8	34.801	31.363	-10	0	12	35.593	35.294
0	0	8	9.447	8.768	-8	0	12	42.724	65.870
0	0	8	26.167	23.346	-6	0	12	35.427	34.564
0	0	8	55.431	54.212	-4	0	12	37.236	34.347
0	0	8	140.085	134.757	2	0	12	58.699	57.538
0	0	8	11.272	6.385	4	0	12	93.703	96.835
0	0	8	22.533	17.700	6	0	12	75.126	76.763
0	0	8	29.012	26.741	12	0	12	117.467	115.443
0	0	8	82.772	78.429	-13	0	13	55.939	56.492
0	0	8	21.350	16.067	-11	0	13	19.435	18.964
0	0	9	74.280	72.349	-9	0	13	170.061	165.062
0	0	9	75.244	70.977	-7	0	13	79.346	76.485
0	0	9	150.683	143.592	-5	0	13	57.207	54.382
0	0	9	146.370	140.511	-1	0	13	77.862	81.373
0	0	9	41.516	39.127	1	0	13	73.081	68.032
0	0	9	21.833	17.275	3	0	13	15.394	14.287
0	0	9	29.423	27.332	5	0	13	23.455	22.786
0	0	9	17.061	19.762	7	0	13	37.077	36.598
0	0	9	17.175	16.534	9	0	13	47.041	41.416
0	0	9	74.228	73.936	-10	0	14	54.500	53.639
0	0	9	99.252	95.997	-8	0	14	38.167	35.307
0	0	9	48.699	48.021	-6	0	14	23.171	21.839
0	0	9	43.309	48.027	-4	0	14	18.320	16.182
0	0	9	87.780	82.523	-2	0	14	26.500	18.566
0	10	34.276	32.233	0	0	14	97.175	94.033	

Gantaclarait Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	0	14	78.362	77.499	18	2	0	20.614	20.646
4	0	14	58.488	56.638	-20	3	0	36.252	37.251
6	0	14	18.134	15.134	-18	3	0	22.411	21.014
8	0	14	44.711	45.184	-16	3	0	23.382	25.005
-7	0	15	17.992	19.383	-14	3	0	24.606	28.087
-5	0	15	58.996	56.758	-12	3	0	55.439	53.825
-3	0	15	46.114	44.078	-10	3	0	20.622	18.666
-1	0	15	118.423	115.080	-8	3	0	15.407	18.433
1	0	15	33.081	30.860	-6	3	0	53.809	58.112
5	0	15	22.841	26.712	-4	3	0	28.947	29.972
2	0	0	125.642	114.011	-2	3	0	30.276	32.900
4	0	0	179.154	169.645	0	3	0	51.049	51.615
8	0	0	52.821	49.526	2	3	0	35.598	36.947
10	0	0	42.919	39.380	4	3	0	74.000	67.265
14	0	0	57.528	59.158	6	3	0	287.837	286.302
16	0	0	27.321	24.295	8	3	0	196.272	201.406
18	0	0	30.846	27.280	10	3	0	139.780	139.059
-20	1	0	20.805	25.187	12	3	0	30.565	29.519
-18	1	0	55.272	56.447	14	3	0	52.829	52.214
-14	1	0	30.126	32.714	16	3	0	34.801	35.087
-12	1	0	19.618	11.249	18	3	0	16.443	17.968
-10	1	0	20.650	21.697	-20	4	0	60.955	56.922
-8	1	0	18.280	11.958	-18	4	0	46.565	44.094
-6	1	0	105.224	102.972	-16	4	0	27.098	30.463
-4	1	0	45.679	45.804	-14	4	0	60.431	59.607
0	1	0	172.532	169.728	-10	4	0	89.752	89.605
2	1	0	157.967	173.602	-8	4	0	12.195	1.244
4	1	0	368.528	362.193	-6	4	0	14.321	13.452
6	1	0	54.898	55.275	-2	4	0	96.354	100.418
8	1	0	9.008	3.029	0	4	0	17.813	23.412
10	1	0	91.805	88.336	2	4	0	29.012	25.641
12	1	0	46.431	49.012	4	4	0	29.012	29.339
14	1	0	27.618	29.536	6	4	0	131.752	136.768
18	1	0	48.260	43.154	8	4	0	209.154	211.518
20	1	0	30.980	28.443	10	4	0	65.955	65.276
20	2	0	22.829	22.670	16	4	0	129.333	126.926
18	2	0	48.272	46.541	18	4	0	19.992	17.025
14	2	0	43.963	41.723	-20	5	0	82.785	79.362
12	2	0	19.537	13.548	-18	5	0	133.695	129.277
10	2	0	24.622	35.972	-16	5	0	42.663	44.792
-8	2	0	41.886	39.641	-12	5	0	46.386	44.207
-6	2	0	19.020	23.274	-10	5	0	97.451	95.511
-4	2	0	28.650	29.189	-8	5	0	15.362	17.196
-2	2	0	47.984	47.848	-6	5	0	21.337	21.474
0	2	0	168.797	166.225	-4	5	0	74.244	73.593
2	2	0	311.496	302.810	-2	5	0	49.878	54.366
4	2	0	120.073	129.327	0	5	0	93.081	97.092
6	2	0	96.077	92.220	2	5	0	133.333	141.330
8	2	0	26.106	30.547	6	5	0	17.610	20.645
10	2	0	9.321	7.620	8	5	0	55.935	56.573
12	2	0	105.020	106.345	10	5	0	165.280	163.707
14	2	0	38.728	36.850	12	5	0	70.199	71.206
16	2	0	59.585	57.675	14	5	0	33.976	32.013

Santaclarite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
16	5	0	17.358	9.782	-6	1	-14	127.215	130.090
-18	6	0	70.126	66.776	-4	1	-14	23.004	21.989
-16	6	0	84.240	79.795	0	1	-14	40.304	41.543
-14	6	0	50.272	50.647	2	1	-14	122.841	125.635
-12	6	0	43.890	46.751	4	1	-14	67.130	66.483
-10	6	0	83.606	84.444	6	1	-14	39.927	41.350
-2	6	0	23.110	22.869	10	1	-14	47.402	44.627
0	6	0	47.565	46.606	-13	1	-13	49.427	48.198
2	6	0	19.329	19.930	-11	1	-13	102.602	105.877
4	6	0	24.785	27.369	-9	1	-13	91.593	96.362
10	6	0	81.809	83.392	-7	1	-13	29.980	30.281
14	6	0	29.524	31.429	-5	1	-13	13.309	14.184
-18	7	0	96.276	94.675	-3	1	-13	51.772	51.962
-16	7	0	87.516	82.333	-1	1	-13	15.955	17.582
-14	7	0	117.634	116.549	1	1	-13	49.748	49.565
-10	7	0	16.524	15.447	3	1	-13	95.411	95.018
-8	7	0	53.467	51.536	7	1	-13	66.049	65.394
-6	7	0	114.801	115.434	9	1	-13	90.439	88.515
-4	7	0	39.451	38.596	11	1	-13	89.236	87.440
-2	7	0	79.541	79.558	13	1	-13	16.642	11.549
0	7	0	18.419	18.844	-14	1	-12	33.630	34.367
4	7	0	103.467	106.307	-12	1	-12	102.260	103.237
6	7	0	33.858	36.319	-10	1	-12	91.500	93.153
8	7	0	31.106	28.736	-8	1	-12	25.646	25.186
10	7	0	26.463	24.494	-4	1	-12	14.439	13.344
12	7	0	38.553	35.888	-2	1	-12	83.065	82.927
-16	8	0	59.341	58.957	0	1	-12	91.431	95.188
-14	8	0	99.728	97.376	2	1	-12	79.862	82.184
-12	8	0	125.740	125.490	4	1	-12	26.179	23.999
-10	8	0	13.171	6.294	6	1	-12	34.606	35.424
-8	8	0	21.740	20.313	8	1	-12	25.622	25.653
-6	8	0	102.585	105.339	10	1	-12	61.858	60.032
-4	8	0	57.041	56.176	12	1	-12	34.244	33.401
0	8	0	38.041	32.79	14	1	-12	13.122	13.682
2	8	0	36.886	33.578	-15	1	-11	29.154	25.843
6	8	0	12.150	9.397	-11	1	-11	106.382	102.595
8	8	0	79.996	84.453	-9	1	-11	45.748	44.368
10	8	0	50.858	50.232	-7	1	-11	32.911	29.628
-2	10	0	67.175	67.609	-5	1	-11	50.780	50.494
-4	1	-16	60.183	55.708	-3	1	-11	172.630	169.740
-2	1	-16	20.089	18.772	-1	1	-11	70.232	67.652
0	1	-16	21.228	25.332	1	1	-11	11.020	10.918
2	1	-16	24.821	25.021	3	1	-11	10.748	2.134
-7	1	-15	64.325	62.738	7	1	-11	14.069	11.588
-5	1	-15	23.329	24.389	9	1	-11	79.402	78.959
-3	1	-15	23.443	20.129	11	1	-11	40.524	39.122
-1	1	-15	23.858	21.765	13	1	-11	75.142	73.938
1	1	-15	18.427	14.138	-16	1	-10	93.896	95.285
3	1	-15	69.065	67.425	-14	1	-10	16.045	13.149
5	1	-15	67.081	65.002	-12	1	-10	13.911	12.754
7	1	-15	25.561	22.874	-10	1	-10	14.146	5.780
9	1	-15	24.634	24.625	-8	1	-10	41.691	39.387
-10	1	-14	71.374	73.829	-6	1	-10	34.772	33.022

Santaclarita Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	1	-10	103.317	99.675	9	1	-7	29.561	28.515
0	1	-10	20.203	20.068	13	1	-7	31.057	20.803
2	1	-10	66.683	66.016	15	1	-7	102.098	99.487
4	1	-10	19.707	18.812	17	1	-7	29.618	20.768
6	1	-10	145.695	142.343	-20	1	-6	80.841	77.248
8	1	-10	80.732	77.759	-18	1	-6	94.256	89.233
10	1	-10	40.256	42.741	-16	1	-6	13.931	10.089
12	1	-10	41.016	42.828	-14	1	-6	22.687	23.412
16	1	-10	45.077	42.755	-12	1	-6	47.976	47.643
-17	1	-9	38.163	38.963	-10	1	-6	45.130	40.584
-15	1	-9	82.699	81.287	-8	1	-6	31.715	32.528
-13	1	-9	122.305	118.762	-6	1	-6	97.931	93.468
-11	1	-9	22.333	21.064	-4	1	-6	31.902	32.172
-9	1	-9	41.159	40.983	-2	1	-6	32.504	35.222
-7	1	-9	93.374	94.736	0	1	-6	38.175	40.637
-5	1	-9	96.037	100.513	4	1	-6	50.939	48.483
-3	1	-9	114.423	115.236	6	1	-6	27.972	24.369
-1	1	-9	16.320	15.495	8	1	-6	50.776	48.891
1	1	-9	31.707	27.934	10	1	-6	367.910	361.429
3	1	-9	10.313	6.692	12	1	-6	78.386	74.704
5	1	-9	70.748	69.375	14	1	-6	99.362	98.631
7	1	-9	18.955	15.614	16	1	-6	18.077	17.182
13	1	-9	50.248	47.541	18	1	-6	18.220	15.997
15	1	-9	82.902	78.963	20	1	-6	48.370	44.599
17	1	-9	81.943	78.514	-19	1	-5	68.663	65.014
-16	1	-8	15.752	9.068	-15	1	-5	28.000	26.080
-14	1	-8	63.854	61.841	-13	1	-5	58.695	56.243
-12	1	-8	38.280	39.587	-11	1	-5	76.354	69.217
-10	1	-8	51.675	51.189	-9	1	-5	154.484	151.864
-8	1	-8	247.894	246.263	-7	1	-5	33.911	32.917
-6	1	-8	231.789	228.108	-5	1	-5	10.102	14.147
-4	1	-8	96.150	94.813	-3	1	-5	8.955	6.185
-2	1	-8	85.183	83.612	-1	1	-5	7.016	2.570
0	1	-8	31.240	28.917	1	1	-5	9.317	13.040
2	1	-8	53.362	54.252	3	1	-5	58.154	56.079
4	1	-8	67.390	68.361	5	1	-5	51.435	47.941
6	1	-8	186.691	184.260	7	1	-5	30.069	31.592
8	1	-8	36.098	33.406	9	1	-5	75.419	78.042
14	1	-8	36.411	34.647	11	1	-5	38.858	41.985
16	1	-8	22.516	25.176	13	1	-5	23.882	23.683
18	1	-8	42.325	40.731	15	1	-5	84.976	83.526
-17	1	-7	87.008	86.612	17	1	-5	57.150	55.623
-15	1	-7	21.927	17.782	19	1	-5	120.077	118.088
-11	1	-7	12.907	15.077	-18	1	-4	17.081	13.756
-9	1	-7	40.915	41.565	-16	1	-4	15.602	12.281
-7	1	-7	54.150	49.961	-14	1	-4	72.012	73.137
-5	1	-7	93.797	92.773	-12	1	-4	9.679	11.828
-3	1	-7	106.289	106.185	-10	1	-4	44.276	42.536
-1	1	-7	43.057	38.997	-8	1	-4	13.915	12.203
1	1	-7	502.410	508.141	-6	1	-4	53.650	52.865
3	1	-7	311.890	304.380	-4	1	-4	76.492	81.187
5	1	-7	51.659	49.792	-2	1	-4	21.992	25.651
7	1	-7	74.528	70.483	0	1	-4	99.240	106.175

Santaclaraite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	1	-4	90.894	88.824	-7	1	-1	459.967	459.533
4	1	-4	26.805	27.290	-5	1	-1	412.378	404.245
6	1	-4	54.927	51.498	-3	1	-1	75.687	72.889
8	1	-4	55.703	55.288	1	1	-1	61.163	73.244
10	1	-4	14.715	8.079	3	1	-1	25.707	24.438
12	1	-4	28.846	26.545	5	1	-1	51.134	46.810
14	1	-4	33.093	36.548	9	1	-1	49.341	46.595
16	1	-4	28.610	27.833	13	1	-1	134.858	129.166
18	1	-4	38.028	38.110	15	1	-1	26.171	26.187
20	1	-4	13.878	16.333	17	1	-1	35.366	38.770
-19	1	-3	53.110	55.193	19	1	-1	37.240	39.792
-17	1	-3	11.427	12.026	21	1	-1	24.724	22.156
-15	1	-3	17.110	14.382	-21	1	1	81.764	78.943
-13	1	-3	131.890	135.009	-19	1	1	82.931	81.179
-9	1	-3	36.854	36.023	-17	1	1	56.276	50.889
-7	1	-3	20.402	23.644	-15	1	1	55.602	54.938
-5	1	-3	68.516	65.728	-13	1	1	14.289	15.169
-3	1	-3	11.488	10.591	-11	1	1	31.146	24.821
-1	1	-3	70.793	80.109	-9	1	1	33.126	37.097
1	1	-3	89.346	89.130	-7	1	1	22.817	25.622
3	1	-3	14.545	15.261	-5	1	1	10.028	6.043
5	1	-3	336.565	327.265	-3	1	1	92.264	76.438
7	1	-3	209.541	203.440	-1	1	1	33.154	35.044
9	1	-3	86.435	83.195	1	1	1	19.175	14.413
11	1	-3	55.073	53.144	3	1	1	10.033	8.649
13	1	-3	56.447	53.670	5	1	1	38.419	26.912
15	1	-3	99.667	96.614	7	1	1	8.581	1.386
17	1	-3	28.313	29.814	9	1	1	265.732	264.301
19	1	-3	30.516	31.127	11	1	1	36.232	35.572
-20	1	-2	37.402	33.916	13	1	1	45.935	43.631
-18	1	-2	86.809	82.111	15	1	1	17.280	17.126
-16	1	-2	111.593	105.485	17	1	1	46.451	47.987
-14	1	-2	272.419	263.425	19	1	1	56.264	53.383
-12	1	-2	10.854	9.274	21	1	1	57.789	60.060
-10	1	-2	21.252	24.139	-20	1	2	17.496	13.293
-8	1	-2	18.024	17.502	-18	1	2	57.089	58.265
-6	1	-2	72.598	65.766	-16	1	2	32.431	23.421
-4	1	-2	159.626	149.626	-14	1	2	164.496	163.071
-2	1	-2	60.923	49.454	-12	1	2	110.833	105.601
0	1	-2	39.427	8.643	-10	1	2	240.427	239.493
2	1	-2	48.728	41.272	-8	1	2	83.260	82.560
4	1	-2	77.715	78.277	-6	1	2	16.972	11.207
6	1	-2	12.728	14.617	-4	1	2	16.171	12.367
8	1	-2	49.931	52.321	-2	1	2	32.951	30.676
10	1	-2	41.138	41.869	0	1	2	81.817	81.715
12	1	-2	33.504	34.556	2	1	2	24.488	25.939
14	1	-2	263.211	257.633	4	1	2	22.634	21.647
16	1	-2	110.289	107.979	6	1	2	64.589	57.188
18	1	-2	89.228	87.070	8	1	2	37.776	35.354
20	1	-2	23.894	17.390	18	1	2	99.402	94.472
-21	1	-1	22.850	23.036	20	1	2	39.264	39.837
-15	1	-1	114.390	111.437	-19	1	3	15.890	14.026
-9	1	-1	27.028	21.739	-17	1	3	44.862	43.720

Santaclarite Structure Factor Table (based on K-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-15	1	3	12.451	12.843	17	1	5	66.874	65.368
-13	1	3	18.939	19.150	19	1	5	17.528	17.471
-11	1	3	28.866	27.235	-20	1	6	47.484	44.817
-9	1	3	9.142	0.899	-18	1	6	15.337	8.583
-7	1	3	69.825	63.772	-16	1	6	31.171	28.336
-5	1	3	49.443	47.447	-12	1	6	31.598	29.788
-3	1	3	265.000	259.882	-10	1	6	125.752	124.290
-1	1	3	497.223	495.690	-8	1	6	260.801	260.158
1	1	3	122.508	119.499	-6	1	6	240.955	237.591
3	1	3	58.870	60.034	-4	1	6	47.041	44.600
5	1	3	99.825	100.710	-2	1	6	12.894	13.943
7	1	3	66.606	66.889	0	1	6	12.801	10.399
9	1	3	18.577	18.456	2	1	6	102.240	105.793
11	1	3	26.439	21.149	4	1	6	46.862	46.108
13	1	3	11.923	6.706	6	1	6	55.333	51.843
15	1	3	48.947	45.443	12	1	6	15.211	7.711
17	1	3	28.285	25.805	14	1	6	47.533	50.055
-20	1	4	40.736	39.836	16	1	6	82.675	86.475
-18	1	4	20.911	17.035	18	1	6	19.435	23.536
-14	1	4	33.024	36.385	-19	1	7	51.327	50.230
-12	1	4	49.890	50.767	-17	1	7	20.130	18.807
-8	1	4	14.024	15.604	-13	1	7	71.285	67.805
-6	1	4	193.813	196.555	-11	1	7	44.012	43.713
-4	1	4	112.557	115.595	-9	1	7	90.167	91.730
-2	1	4	87.069	87.086	-7	1	7	66.049	63.500
0	1	4	44.496	43.436	-5	1	7	22.565	23.021
2	1	4	33.724	30.788	-3	1	7	28.272	25.767
4	1	4	69.577	68.711	-1	1	7	22.187	18.041
6	1	4	300.719	296.737	1	1	7	152.289	151.636
8	1	4	347.297	346.583	3	1	7	160.191	163.773
10	1	4	76.500	74.732	5	1	7	105.496	100.970
12	1	4	76.053	78.402	9	1	7	47.744	48.857
14	1	4	99.760	96.899	11	1	7	94.228	94.146
16	1	4	31.951	29.499	13	1	7	21.764	22.972
20	1	4	27.553	31.186	15	1	7	52.691	51.784
-19	1	5	78.415	77.247	17	1	7	35.935	37.728
-17	1	5	151.419	144.829	-18	1	8	142.488	136.694
-15	1	5	149.496	141.505	-16	1	8	23.602	20.368
-13	1	5	105.732	100.491	-14	1	8	21.337	18.891
-11	1	5	11.346	11.560	-12	1	8	47.984	44.304
-9	1	5	28.130	29.174	-10	1	8	32.821	29.071
-7	1	5	98.321	96.035	-8	1	8	15.045	12.666
-5	1	5	62.565	57.547	-6	1	8	25.098	24.045
-3	1	5	7.805	3.373	-4	1	8	134.411	132.704
-1	1	5	36.378	29.468	-2	1	8	69.492	73.511
1	1	5	17.362	14.892	0	1	8	130.549	131.967
3	1	5	48.110	51.927	2	1	8	49.484	50.394
5	1	5	60.813	66.384	4	1	8	17.232	15.332
7	1	5	122.114	124.317	6	1	8	51.467	54.399
9	1	5	56.809	54.620	8	1	8	24.126	23.766
11	1	5	18.846	22.123	10	1	8	74.606	74.854
13	1	5	131.427	129.039	12	1	8	103.683	101.622
15	1	5	114.756	110.749	14	1	8	65.447	67.627



Santaclarite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
16	1	8	16.846	10.398	3	1	13	25.370	24.349
-17	1	9	31.553	32.136	5	1	13	36.354	38.693
-15	1	9	20.150	18.844	7	1	13	23.772	23.936
-11	1	9	96.045	92.479	9	1	13	7.301 *	3.197
-9	1	9	134.906	131.339	-8	1	14	21.057	18.108
-7	1	9	50.728	49.943	-6	1	14	57.028	54.685
-5	1	9	42.634	42.252	-4	1	14	15.854	16.840
-3	1	9	142.463	140.544	2	1	14	38.167	37.526
-1	1	9	67.569	66.731	4	1	14	60.285	60.428
1	1	9	60.012	61.497	6	1	14	16.467	16.803
3	1	9	42.423	41.634	-5	1	15	43.748	38.178
5	1	9	12.752	7.850	-3	1	15	31.362	27.951
7	1	9	42.150	44.451	-1	1	15	28.106	17.469
9	1	9	101.289	105.481	1	1	15	18.947	16.151
11	1	9	57.406	59.666	3	1	15	85.675	84.990
15	1	9	29.236	32.402	-6	2	-16	61.146	61.808
-14	1	10	16.577	17.052	-4	2	-16	46.341	47.212
-10	1	10	68.687	69.200	-2	2	-16	43.443	41.450
-6	1	10	34.630	32.810	2	2	-16	33.439	28.993
-4	1	10	126.163	125.593	4	2	-16	16.329	9.340
-2	1	10	179.846	177.555	-9	2	-15	43.646	45.598
0	1	10	39.419	39.057	-7	2	-15	54.805	55.072
4	1	10	56.264	55.764	-5	2	-15	143.703	145.715
6	1	10	125.736	126.195	-3	2	-15	106.557	104.633
8	1	10	41.146	38.085	-1	2	-15	68.329	67.402
10	1	10	60.016	58.325	1	2	-15	18.675	19.669
12	1	10	36.354	33.815	3	2	-15	64.492	63.480
14	1	10	64.874	60.775	5	2	-15	76.133	77.278
-15	1	11	57.480	54.288	7	2	-15	93.862	89.660
-11	1	11	31.350	22.089	9	2	-15	25.179	28.432
-9	1	11	26.150	27.340	-12	2	-14	13.935	16.923
-5	1	11	50.077	51.508	-6	2	-14	18.585	19.090
-1	1	11	37.415	37.758	-4	2	-14	62.431	61.283
1	1	11	30.439	27.685	0	2	-14	26.610	23.668
3	1	11	24.972	24.650	2	2	-14	129.594	126.872
5	1	11	122.378	121.945	4	2	-14	174.427	175.455
7	1	11	115.545	113.224	6	2	-14	35.752	33.430
13	1	11	68.463	67.470	8	2	-14	56.346	54.522
-14	1	12	122.073	116.099	-11	2	-13	49.732	48.028
-12	1	12	14.199	16.721	-9	2	-13	37.423	36.200
-10	1	12	20.593	20.514	-5	2	-13	42.065	39.754
-8	1	12	71.687	71.405	-3	2	-13	29.976	29.255
-6	1	12	38.028	36.919	1	2	-13	25.878	25.234
0	1	12	60.533	59.139	3	2	-13	32.191	33.722
2	1	12	21.443	20.423	5	2	-13	21.980	19.071
4	1	12	131.492	126.915	7	2	-13	20.179	17.477
8	1	12	20.049	18.568	11	2	-13	170.748	172.755
12	1	12	27.951	30.003	13	2	-13	116.427	114.940
-11	1	13	37.232	36.983	-14	2	-12	28.654	29.280
-9	1	13	28.089	29.363	-10	2	-12	52.630	54.043
-7	1	13	17.309	8.581	-8	2	-12	72.459	69.586
-5	1	13	139.293	137.961	-6	2	-12	18.264	16.989
1	1	13	62.419	60.660	-4	2	-12	23.789	25.138

Santaclaraite Structure Factor Table (based on K-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	2	-12	37.508	36.511	-18	2	-8	36.520	32.442
0	2	-12	33.159	30.940	-16	2	-8	15.427	13.885
2	2	-12	41.350	40.989	-14	2	-8	79.012	75.716
4	2	-12	39.520	39.072	-12	2	-8	83.476	82.035
6	2	-12	41.736	42.934	-10	2	-8	10.459	10.296
8	2	-12	24.325	22.038	-8	2	-8	71.390	73.519
10	2	-12	28.297	27.225	-6	2	-8	120.772	117.381
12	2	-12	30.809	30.016	-4	2	-8	373.589	370.930
-15	2	-11	28.894	27.167	-2	2	-8	46.618	47.849
-13	2	-11	60.589	61.585	0	2	-8	9.541	7.006
-11	2	-11	37.146	37.796	2	2	-8	24.589	23.039
-9	2	-11	28.102	26.065	4	2	-8	10.228	11.763
-7	2	-11	52.236	51.805	6	2	-8	27.524	26.657
-3	2	-11	63.146	64.796	8	2	-8	39.667	40.423
-1	2	-11	81.069	77.425	10	2	-8	91.841	91.305
1	2	-11	82.423	79.076	14	2	-8	38.927	38.458
3	2	-11	31.846	31.099	16	2	-8	52.447	53.216
5	2	-11	22.715	21.805	18	2	-8	45.866	43.785
7	2	-11	23.923	26.756	-17	2	-7	89.963	90.095
11	2	-11	70.439	67.717	-15	2	-7	58.394	54.484
13	2	-11	25.606	24.786	-13	2	-7	48.764	44.023
15	2	-11	24.553	20.537	-11	2	-7	18.902	22.051
-16	2	-10	20.923	22.080	-9	2	-7	40.760	40.346
-14	2	-10	57.508	52.993	-7	2	-7	9.150	10.168
-12	2	-10	153.947	158.542	-5	2	-7	84.175	87.499
-10	2	-10	42.102	41.133	-3	2	-7	37.419	38.216
-8	2	-10	55.179	59.116	1	2	-7	34.504	35.835
-6	2	-10	24.573	24.633	3	2	-7	111.028	108.093
-4	2	-10	56.785	55.942	5	2	-7	225.602	223.173
-2	2	-10	18.053	13.012	9	2	-7	25.447	24.959
0	2	-10	22.711	20.198	11	2	-7	23.224	21.737
2	2	-10	76.073	75.654	17	2	-7	56.715	54.218
4	2	-10	53.069	51.042	19	2	-7	57.004	56.161
6	2	-10	121.866	119.971	-20	2	-6	27.782	23.485
8	2	-10	135.594	133.412	-18	2	-6	58.858	59.708
10	2	-10	52.801	53.958	-16	2	-6	77.923	72.710
12	2	-10	48.841	46.351	-14	2	-6	79.370	76.175
16	2	-10	56.325	51.672	-12	2	-6	41.138	45.682
-17	2	-9	67.650	66.827	-8	2	-6	131.045	134.571
-15	2	-9	49.346	47.500	-6	2	-6	31.333	31.110
-13	2	-9	185.715	184.188	-4	2	-6	122.841	123.143
-11	2	-9	82.614	81.980	0	2	-6	12.293	12.925
-7	2	-9	79.211	78.118	2	2	-6	20.081	19.607
-5	2	-9	95.699	94.217	4	2	-6	33.382	34.138
-3	2	-9	129.589	131.878	6	2	-6	53.134	52.593
-1	2	-9	69.837	69.894	10	2	-6	108.337	108.216
1	2	-9	62.541	62.793	12	2	-6	47.451	43.937
3	2	-9	11.289	9.142	14	2	-6	72.028	71.905
5	2	-9	57.768	57.351	16	2	-6	36.752	34.772
9	2	-9	74.524	76.379	18	2	-6	15.451	7.074
13	2	-9	11.886	9.805	-21	2	-5	29.118	24.398
15	2	-9	139.780	136.273	-17	2	-5	59.415	56.664
17	2	-9	123.569	119.828	-15	2	-5	35.435	34.694

Santaclarite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-13	2	-5	123.004	121.116	-18	2	-2	81.710	82.300
-11	2	-5	12.870	9.111	-16	2	-2	65.585	64.747
-9	2	-5	222.772	222.069	-14	2	-2	211.911	200.888
-7	2	-5	150.020	148.057	-12	2	-2	151.969	141.026
-3	2	-5	42.406	41.882	-10	2	-2	92.659	93.693
-1	2	-5	49.595	47.767	-8	2	-2	61.890	61.745
1	2	-5	39.256	31.107	-6	2	-2	37.382	27.727
3	2	-5	119.906	116.908	-4	2	-2	65.711	67.977
5	2	-5	118.581	118.347	-2	2	-2	138.976	132.148
7	2	-5	15.130	12.228	0	2	-2	20.963	22.296
9	2	-5	10.846	10.085	2	2	-2	30.203	28.834
11	2	-5	14.602	17.206	4	2	-2	48.886	52.918
13	2	-5	26.691	27.153	6	2	-2	28.710	27.597
15	2	-5	13.683	14.263	8	2	-2	109.606	112.478
17	2	-5	26.398	25.012	10	2	-2	69.435	68.395
19	2	-5	96.114	91.314	12	2	-2	20.557	25.547
-18	2	-4	57.435	53.086	14	2	-2	112.858	112.159
-16	2	-4	12.833	15.954	16	2	-2	102.764	99.943
-14	2	-4	26.886	28.352	18	2	-2	126.171	120.497
-10	2	-4	19.923	14.869	-21	2	-1	34.756	31.184
-8	2	-4	63.581	63.497	-19	2	-1	47.179	44.904
-6	2	-4	73.057	73.875	-17	2	-1	18.963	19.373
-4	2	-4	77.183	77.641	-15	2	-1	14.768	17.153
-2	2	-4	166.484	157.776	-13	2	-1	37.423	33.777
0	2	-4	564.878	586.283	-11	2	-1	54.528	54.813
2	2	-4	104.768	101.347	-9	2	-1	208.740	210.487
4	2	-4	121.195	118.454	-7	2	-1	157.780	151.383
6	2	-4	40.293	39.844	-5	2	-1	310.294	303.068
8	2	-4	96.512	95.120	-3	2	-1	87.545	99.910
12	2	-4	21.020	23.559	-1	2	-1	50.817	49.105
14	2	-4	51.980	53.400	1	2	-1	109.346	114.349
16	2	-4	12.524	4.395	3	2	-1	128.606	131.592
18	2	-4	18.085	15.658	7	2	-1	8.484	0.930
-21	2	-3	176.150	167.056	9	2	-1	28.654	26.034
-19	2	-3	68.268	63.552	11	2	-1	25.224	20.407
-17	2	-3	20.280	17.955	17	2	-1	89.854	92.012
-15	2	-3	17.740	16.496	-21	2	1	30.207	32.372
-13	2	-3	59.378	64.327	-19	2	1	79.915	76.090
-11	2	-3	52.191	51.268	-17	2	1	170.866	164.962
-9	2	-3	30.947	27.101	-15	2	1	150.293	143.406
-7	2	-3	56.431	52.265	-13	2	1	56.817	56.579
-3	2	-3	62.167	59.027	-11	2	1	37.061	39.001
-1	2	-3	18.695	25.517	-9	2	1	57.411	56.759
1	2	-3	16.557	16.584	-7	2	1	36.801	36.043
3	2	-3	28.772	28.359	-5	2	1	42.126	39.274
5	2	-3	59.618	55.947	-3	2	1	130.301	116.406
7	2	-3	212.317	204.879	-1	2	1	83.813	82.620
9	2	-3	470.736	466.561	1	2	1	95.890	92.267
11	2	-3	35.187	20.196	3	2	1	72.841	78.257
13	2	-3	103.175	104.279	5	2	1	9.541	12.291
15	2	-3	25.512	21.025	7	2	1	47.980	49.439
17	2	-3	62.915	60.636	11	2	1	47.073	47.095
-20	2	-2	35.060	17.107	13	2	1	228.825	228.521

Santaclaraite Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
15	2	1	56.638	54.103	10	2	4	21.472	22.112
17	2	1	82.337	81.738	12	2	4	57.776	58.435
19	2	1	36.606	35.431	14	2	4	32.419	31.194
-18	2	2	20.439	22.987	16	2	4	67.598	63.513
-16	2	2	23.463	22.365	18	2	4	35.346	34.835
-12	2	2	37.980	40.314	-17	2	5	74.126	71.984
-10	2	2	46.077	42.411	-15	2	5	73.012	70.553
-8	2	2	330.557	323.896	-13	2	5	222.638	220.760
-6	2	2	126.894	127.932	-11	2	5	98.797	96.450
-4	2	2	68.545	68.611	-9	2	5	35.041	33.771
-2	2	2	117.593	120.504	-7	2	5	35.455	36.641
0	2	2	108.110	111.295	-5	2	5	40.886	42.199
2	2	2	42.077	37.796	-3	2	5	44.805	43.996
4	2	2	69.187	65.949	-1	2	5	66.004	64.674
6	2	2	25.366	23.768	1	2	5	22.069	21.820
8	2	2	13.110	15.739	3	2	5	122.789	124.994
10	2	2	76.000	74.438	5	2	5	156.232	156.791
12	2	2	96.882	98.594	7	2	5	42.346	43.694
14	2	2	17.228	13.695	9	2	5	24.947	20.962
16	2	2	40.809	44.665	15	2	5	59.512	59.245
18	2	2	49.878	49.670	17	2	5	98.569	97.400
-21	2	3	27.841	29.852	-20	2	6	28.793	27.911
-19	2	3	28.467	28.805	-18	2	6	35.606	35.014
-17	2	3	15.354	13.758	-14	2	6	14.598	16.317
-15	2	3	11.228	2.078	-12	2	6	19.520	19.122
-13	2	3	65.065	66.982	-10	2	6	23.069	21.880
-11	2	3	21.224	22.095	-8	2	6	11.512	11.475
-9	2	3	34.382	36.363	-6	2	6	129.675	130.800
-7	2	3	32.894	32.435	-4	2	6	233.297	234.226
-5	2	3	100.951	99.690	-2	2	6	120.890	121.733
-3	2	3	83.293	85.361	0	2	6	86.882	86.587
-1	2	3	414.650	406.970	2	2	6	84.102	85.654
1	2	3	303.345	298.053	4	2	6	52.272	50.981
3	2	3	70.122	73.873	6	2	6	35.565	38.834
5	2	3	77.736	79.699	8	2	6	30.280	30.505
7	2	3	140.821	143.249	10	2	6	21.703	21.474
9	2	3	99.614	97.442	14	2	6	76.447	72.913
11	2	3	31.337	32.202	16	2	6	14.687	18.092
13	2	3	29.593	27.250	-19	2	7	32.817	32.979
15	2	3	42.821	41.313	-15	2	7	14.923	12.267
19	2	3	61.549	62.697	-9	2	7	54.358	52.820
-20	2	4	62.837	60.294	-7	2	7	64.988	66.184
-18	2	4	19.618	15.302	-5	2	7	106.463	109.022
-16	2	4	34.028	34.410	-3	2	7	17.931	15.667
-14	2	4	60.130	60.601	-1	2	7	19.236	16.467
-12	2	4	25.242	20.596	1	2	7	13.154	14.861
-10	2	4	80.740	82.713	3	2	7	35.028	31.800
-4	2	4	28.825	27.562	5	2	7	145.085	147.713
0	2	4	40.163	46.212	7	2	7	74.244	75.153
2	2	4	37.476	35.528	9	2	7	65.358	64.788
4	2	4	50.638	48.893	11	2	7	77.850	77.834
6	2	4	127.394	130.256	13	2	7	54.906	54.896
8	2	4	248.821	245.373	15	2	7	25.350	25.492

Santaclarite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
17	2	7	17.537	16.488	5	2	11	33.297	35.779
-18	2	8	147.963	143.235	7	2	11	25.707	22.228
-16	2	8	106.146	101.971	9	2	11	75.207	76.676
-14	2	8	73.467	73.161	11	2	11	33.524	36.320
-12	2	8	31.614	30.937	-12	2	12	49.789	47.406
-10	2	8	44.187	45.551	-10	2	12	21.004	21.901
-8	2	8	70.557	67.445	-8	2	12	36.392	26.121
-6	2	8	9.882	13.485	-6	2	12	36.992	37.723
-4	2	8	46.463	44.222	-4	2	12	51.272	53.829
-2	2	8	67.923	68.582	0	2	12	55.801	53.965
0	2	8	28.650	29.939	4	2	12	28.850	33.299
2	2	8	74.776	76.264	6	2	12	37.268	37.620
4	2	8	122.569	130.574	8	2	12	101.467	105.223
6	2	8	43.024	45.548	-9	2	13	19.646	22.033
8	2	8	25.923	22.661	-5	2	13	74.710	73.649
10	2	8	27.984	26.637	-3	2	13	40.634	44.119
12	2	8	96.870	94.144	-1	2	13	17.370	17.181
14	2	8	65.512	67.027	1	2	13	12.207	11.421
16	2	8	31.049	29.015	3	2	13	78.126	77.668
-15	2	9	31.996	29.179	5	2	13	100.504	98.835
-13	2	9	54.028	52.169	7	2	13	26.703	25.059
-11	2	9	19.992	19.216	-6	2	14	44.626	45.042
-9	2	9	249.593	248.151	-4	2	14	20.171	19.136
-7	2	9	126.760	126.057	-2	2	14	38.598	36.946
-5	2	9	33.906	31.226	4	2	14	98.187	101.569
-1	2	9	88.943	88.316	-6	3	-16	28.780	26.788
1	2	9	109.000	107.088	-4	3	-16	28.341	25.928
5	2	9	70.610	69.667	-2	3	-16	75.915	73.825
7	2	9	28.589	28.376	0	3	-16	74.943	74.643
9	2	9	47.504	44.588	2	3	-16	66.236	64.553
11	2	9	16.191	21.844	4	3	-16	14.358	9.276
13	2	9	55.691	59.645	6	3	-16	32.374	31.227
15	2	9	25.850	23.259	-9	3	-15	31.236	32.258
-14	2	10	91.789	91.422	-7	3	-15	23.785	25.788
-12	2	10	29.142	25.915	-5	3	-15	14.289	7.510
-10	2	10	53.923	54.808	-3	3	-15	142.102	143.394
-6	2	10	60.329	61.196	-1	3	-15	93.533	88.915
-4	2	10	33.780	32.952	3	3	-15	56.959	54.222
-2	2	10	62.776	63.362	5	3	-15	39.411	35.207
0	2	10	195.573	194.095	7	3	-15	33.337	35.715
2	2	10	112.569	112.941	9	3	-15	55.033	55.225
4	2	10	103.740	105.402	-12	3	-14	14.159	10.384
6	2	10	46.341	45.380	-10	3	-14	16.528	12.324
8	2	10	83.016	84.773	-8	3	-14	54.037	53.709
10	2	10	22.654	25.069	-6	3	-14	26.170	23.810
12	2	10	25.772	27.997	-4	3	-14	40.398	38.884
-13	2	11	51.557	49.773	-2	3	-14	49.110	49.356
-11	2	11	46.577	43.416	0	3	-14	13.232	11.646
-7	2	11	31.854	29.982	2	3	-14	20.675	15.516
-5	2	11	80.142	81.971	4	3	-14	44.728	44.503
-3	2	11	18.874	17.798	6	3	-14	132.508	127.256
-1	2	11	111.504	112.103	-13	3	-13	56.154	55.857
1	2	11	12.744	5.535	-11	3	-13	51.443	52.094

Santaclarite Structure Factor Table (based on K-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-9	3	-13	19.963	20.016	11	3	-9	17.833	16.281
-7	3	-13	95.024	95.182	15	3	-9	49.037	47.505
-3	3	-13	57.211	58.827	17	3	-9	66.228	65.257
-1	3	-13	27.480	27.097	-16	3	-8	26.756	28.516
1	3	-13	20.549	17.956	-14	3	-8	39.346	39.699
7	3	-13	36.240	20.766	-12	3	-8	10.748	1.999
13	3	-13	48.333	45.680	-10	3	-8	71.034	71.711
-14	3	-12	31.675	30.486	-8	3	-8	81.637	82.776
4	3	-12	34.671	34.075	-6	3	-8	34.750	37.073
6	3	-12	94.959	92.963	-4	3	-8	181.028	175.525
10	3	-12	14.293	17.165	-2	3	-8	88.102	87.065
12	3	-12	29.370	27.743	0	3	-8	51.313	52.693
-17	3	-11	72.488	69.972	2	3	-8	78.626	75.610
-15	3	-11	24.500	25.798	4	3	-8	73.606	74.380
-13	3	-11	15.614	13.602	6	3	-8	22.195	22.510
-11	3	-11	11.793	10.824	8	3	-8	28.256	27.718
-7	3	-11	56.289	56.611	10	3	-8	10.626	6.537
-5	3	-11	48.346	47.392	12	3	-8	11.203	4.522
-3	3	-11	92.833	93.407	14	3	-8	18.837	14.741
1	3	-11	262.061	259.969	18	3	-8	43.492	40.396
3	3	-11	196.988	196.043	-17	3	-7	49.870	47.139
5	3	-11	24.427	23.450	-15	3	-7	20.980	15.844
7	3	-11	99.358	96.983	-13	3	-7	86.541	85.505
9	3	-11	46.179	43.626	-11	3	-7	47.211	47.635
13	3	-11	32.313	32.785	-9	3	-7	17.512	14.975
15	3	-11	104.073	99.752	-7	3	-7	25.801	27.844
-18	3	-10	83.057	77.982	-5	3	-7	92.325	94.812
-14	3	-10	43.154	41.522	-1	3	-7	22.378	23.137
-12	3	-10	54.215	54.762	1	3	-7	89.935	88.084
-10	3	-10	37.508	35.314	3	3	-7	77.988	77.295
-8	3	-10	46.667	45.378	5	3	-7	215.972	215.407
-6	3	-10	27.280	27.733	7	3	-7	23.463	17.650
-4	3	-10	38.772	38.871	9	3	-7	45.846	43.408
-2	3	-10	24.748	27.559	11	3	-7	68.634	66.342
0	3	-10	12.663	9.194	13	3	-7	54.492	52.134
2	3	-10	47.341	47.942	15	3	-7	62.854	61.351
4	3	-10	14.748	16.105	17	3	-7	21.236	19.306
8	3	-10	46.228	46.545	-20	3	-6	13.337	6.901
10	3	-10	263.679	256.805	-18	3	-6	92.329	90.580
12	3	-10	108.142	104.421	-16	3	-6	109.333	104.797
14	3	-10	76.907	73.787	-14	3	-6	171.785	172.909
16	3	-10	13.866	16.957	-8	3	-6	36.081	27.219
-13	3	-9	68.959	67.121	-6	3	-6	98.163	96.761
-11	3	-9	177.785	175.715	-4	3	-6	167.280	168.458
-9	3	-9	84.106	81.181	-2	3	-6	20.744	22.405
-5	3	-9	11.236	11.275	2	3	-6	10.500	10.860
-3	3	-9	159.492	164.086	4	3	-6	54.687	57.833
-1	3	-9	110.256	113.021	8	3	-6	39.691	39.925
1	3	-9	43.496	44.806	10	3	-6	23.516	23.854
3	3	-9	36.390	35.381	12	3	-6	35.431	35.085
5	3	-9	27.110	25.526	14	3	-6	161.813	162.176
7	3	-9	46.813	46.239	16	3	-6	37.203	37.082
9	3	-9	75.931	75.665	18	3	-6	60.366	57.677
					-19	3	-5	18.931	10.504

Santaclarite Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-17	3	-5	14.370	19.273	15	3	-3	14.821	13.062
-15	3	-5	40.679	36.383	17	3	-3	60.224	57.718
-13	3	-5	20.252	20.877	19	3	-3	34.638	31.663
-11	3	-5	40.248	41.859	-20	3	-2	46.492	40.516
-9	3	-5	22.346	22.385	-18	3	-2	72.972	71.224
-7	3	-5	308.459	303.628	-16	3	-2	61.906	59.923
-5	3	-5	286.024	286.803	-14	3	-2	174.787	174.694
-3	3	-5	59.077	59.709	-12	3	-2	201.423	192.996
-1	3	-5	13.354	12.785	-10	3	-2	197.439	195.621
1	3	-5	26.724	30.141	-6	3	-2	22.813	19.809
3	3	-5	66.793	70.571	-4	3	-2	74.244	76.712
5	3	-5	39.508	38.804	-2	3	-2	33.484	32.446
7	3	-5	82.032	79.138	0	3	-2	133.325	131.662
9	3	-5	15.772	15.820	2	3	-2	36.386	39.845
11	3	-5	35.508	35.800	4	3	-2	22.547	21.375
13	3	-5	63.553	64.091	6	3	-2	20.307	18.484
15	3	-5	44.065	41.912	8	3	-2	64.427	65.154
17	3	-5	58.358	61.010	10	3	-2	14.285	15.096
19	3	-5	27.724	26.127	12	3	-2	30.394	28.994
-20	3	-4	34.398	33.969	14	3	-2	37.801	35.567
-18	3	-4	80.874	87.334	16	3	-2	54.663	53.455
-16	3	-4	21.626	22.187	18	3	-2	134.569	133.266
-14	3	-4	46.358	43.409	-17	3	-1	17.419	19.531
-12	3	-4	20.561	15.771	-15	3	-1	11.598	9.319
-10	3	-4	17.301	20.523	-13	3	-1	19.553	18.773
-6	3	-4	65.589	67.463	-11	3	-1	20.260	23.031
-4	3	-4	7.833	6.907	-9	3	-1	41.110	42.523
-2	3	-4	79.285	75.276	-7	3	-1	14.622	10.595
0	3	-4	268.894	270.009	-5	3	-1	146.845	142.066
2	3	-4	382.829	388.808	-3	3	-1	83.959	91.601
4	3	-4	191.980	195.371	-1	3	-1	275.244	278.817
6	3	-4	61.243	59.638	1	3	-1	78.882	77.376
8	3	-4	36.898	37.048	5	3	-1	42.955	44.331
10	3	-4	73.663	72.096	7	3	-1	75.098	73.521
12	3	-4	14.004	15.768	9	3	-1	63.402	62.368
18	3	-4	56.537	55.562	11	3	-1	22.528	19.783
-21	3	-3	121.472	113.878	13	3	-1	14.419	17.051
-19	3	-3	61.480	58.232	15	3	-1	61.378	57.587
-17	3	-3	92.187	87.846	17	3	-1	46.650	47.912
-15	3	-3	12.260	9.680	19	3	-1	21.142	16.745
-13	3	-3	41.024	41.824	-21	3	1	33.093	35.416
-11	3	-3	12.593	11.096	-19	3	1	47.280	45.876
-9	3	-3	122.785	126.581	-17	3	1	121.484	114.901
-7	3	-3	84.276	83.485	-15	3	1	171.098	164.283
-5	3	-3	12.293	7.378	-13	3	1	149.878	145.118
-3	3	-3	19.285	23.387	-11	3	1	19.427	21.120
-1	3	-3	64.528	63.591	-9	3	1	33.955	36.880
1	3	-3	19.646	21.251	-7	3	1	86.951	84.506
5	3	-3	46.154	44.298	-5	3	1	9.976	5.394
7	3	-3	76.663	79.468	-3	3	1	36.809	33.483
9	3	-3	244.081	243.204	-1	3	1	92.650	86.466
11	3	-3	25.244	19.906	1	3	1	25.207	26.109
13	3	-3	64.378	62.754	3	3	1	86.260	88.007

Santaclaraite Structure Factor Table (based on K-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
5	3	1	101.358	106.087	0	3	4	113.183	115.130
7	3	1	60.760	62.485	2	3	4	41.638	46.580
9	3	1	65.053	63.234	4	3	4	17.724	17.767
11	3	1	61.894	63.328	6	3	4	48.467	51.549
13	3	1	54.325	54.252	8	3	4	31.069	31.185
15	3	1	105.602	104.198	10	3	4	113.301	112.994
17	3	1	100.333	97.823	12	3	4	102.228	101.919
19	3	1	39.069	37.972	14	3	4	106.699	106.182
-20	3	2	71.776	71.248	16	3	4	34.041	33.781
-16	3	2	28.293	26.801	18	3	4	61.004	64.719
-12	3	2	96.520	94.324	-17	3	5	26.598	25.498
-10	3	2	87.313	86.206	-13	3	5	23.301	21.424
-8	3	2	387.858	387.102	-11	3	5	18.467	16.619
-6	3	2	378.719	371.424	-9	3	5	149.138	149.792
-4	3	2	17.874	19.267	-7	3	5	20.000	17.701
-2	3	2	67.626	67.953	-5	3	5	16.846	18.063
0	3	2	42.719	46.388	-3	3	5	130.602	131.299
2	3	2	150.167	158.113	-1	3	5	26.382	24.378
4	3	2	25.825	24.026	1	3	5	30.073	28.264
6	3	2	29.841	24.141	3	3	5	51.634	47.408
8	3	2	37.215	37.645	5	3	5	15.715	18.203
10	3	2	18.240	14.295	7	3	5	76.707	81.210
12	3	2	24.126	22.265	9	3	5	110.163	115.092
14	3	2	54.126	55.711	11	3	5	66.719	71.986
16	3	2	54.805	54.575	13	3	5	37.740	39.317
18	3	2	26.630	22.513	15	3	5	57.167	55.631
-21	3	3	20.508	21.573	17	3	5	30.983	28.911
-19	3	3	55.443	52.116	-18	3	6	63.972	62.494
-13	3	3	33.589	32.517	-16	3	6	21.175	17.076
-11	3	3	83.272	85.629	-12	3	6	36.459	39.025
-9	3	3	24.045	23.314	-10	3	6	17.996	16.829
-7	3	3	29.219	33.901	-8	3	6	21.711	19.579
-5	3	3	51.642	53.640	-6	3	6	22.268	20.810
-1	3	3	70.793	64.832	-4	3	6	167.724	168.234
1	3	3	332.923	334.409	-2	3	6	76.809	74.999
3	3	3	227.285	231.338	0	3	6	78.224	80.510
5	3	3	66.902	66.618	2	3	6	39.191	36.380
9	3	3	41.646	40.077	4	3	6	23.496	24.083
11	3	3	91.638	88.423	6	3	6	200.504	204.003
13	3	3	33.012	31.963	8	3	6	13.610	11.943
15	3	3	25.553	27.913	10	3	6	75.244	71.969
17	3	3	13.935	7.976	12	3	6	36.630	37.086
-20	3	4	12.809	12.093	14	3	6	62.744	58.845
-18	3	4	139.520	131.884	16	3	6	18.626	15.525
-16	3	4	17.146	11.842	-17	3	7	66.488	69.718
-14	3	4	26.959	28.086	-15	3	7	37.224	33.690
-12	3	4	33.780	31.532	-11	3	7	35.898	35.542
-10	3	4	104.837	102.804	-9	3	7	63.484	63.284
-8	3	4	13.199	12.587	-7	3	7	20.764	19.826
-6	3	4	16.598	16.791	-5	3	7	25.500	24.327
-4	3	4	145.915	141.720	-3	3	7	61.122	61.760
-2	3	4	19.602	24.168	-1	3	7	72.419	72.576
					1	3	7	14.484	16.393



Santaclarite Structure Factor Table (based on Ii-ce))

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	3	7	35.028	35.401	5	3	11	23.463	23.123
5	3	7	178.142	178.511	9	3	11	12.565	11.346
7	3	7	117.907	119.295	-10	3	12	160.902	162.677
9	3	7	13.935	11.902	-8	3	12	25.537	27.948
11	3	7	15.321	15.349	-4	3	12	11.748	14.526
13	3	7	61.528	62.568	-2	3	12	87.732	85.431
15	3	7	107.110	104.870	0	3	12	34.516	32.960
-16	3	8	56.736	56.981	2	3	12	51.687	52.899
-14	3	8	168.476	168.792	4	3	12	30.317	30.164
-12	3	8	13.159	11.689	6	3	12	62.106	58.276
-8	3	8	96.732	97.984	-7	3	13	37.923	37.708
-6	3	8	88.821	87.997	-3	3	13	85.370	87.262
-4	3	8	10.866	6.971	-1	3	13	106.455	107.612
-2	3	8	77.516	74.422	-6	4	-16	13.573	14.789
0	3	8	48.740	47.711	-2	4	-16	68.817	67.904
2	3	8	41.390	39.042	0	4	-16	26.687	21.215
4	3	8	133.228	135.735	2	4	-16	17.524	20.797
6	3	8	25.679	27.173	6	4	-16	27.898	27.914
8	3	8	22.289	21.650	-7	4	-15	32.191	30.492
14	3	8	71.837	71.475	-3	4	-15	58.650	59.739
-11	3	9	47.516	46.890	-1	4	-15	93.634	90.195
-9	3	9	34.065	34.781	7	4	-15	28.980	28.584
-7	3	9	27.728	27.167	9	4	-15	34.679	33.565
-5	3	9	159.691	157.192	-12	4	-14	79.102	80.946
-3	3	9	17.081	16.224	-10	4	-14	13.053	11.240
-1	3	9	24.000	25.060	-8	4	-14	22.911	23.761
1	3	9	112.679	111.044	-6	4	-14	24.967	22.735
3	3	9	12.711	10.862	-4	4	-14	59.045	58.004
5	3	9	50.801	52.083	0	4	-14	20.488	19.322
9	3	9	28.923	28.106	4	4	-14	22.118	22.603
11	3	9	21.980	17.656	6	4	-14	95.276	94.171
13	3	9	105.004	105.985	8	4	-14	78.520	74.518
-14	3	10	16.801	16.406	-13	4	-13	116.764	114.019
-12	3	10	29.187	25.741	-11	4	-13	51.711	51.326
-10	3	10	49.114	50.284	-9	4	-13	30.683	32.924
-8	3	10	12.707	12.644	-7	4	-13	15.890	16.549
-6	3	10	24.256	25.321	-5	4	-13	73.191	71.793
-4	3	10	14.276	17.188	-3	4	-13	91.520	93.322
-2	3	10	18.142	15.910	-1	4	-13	16.943	18.857
0	3	10	19.768	19.959	1	4	-13	42.020	40.613
2	3	10	14.362	10.856	5	4	-13	23.846	25.104
4	3	10	62.565	66.454	9	4	-13	24.069	24.097
6	3	10	37.024	37.619	-14	4	-12	29.748	27.260
8	3	10	14.065	18.885	-12	4	-12	101.484	99.570
10	3	10	86.260	87.929	-10	4	-12	18.370	21.943
-13	3	11	13.033	10.424	-8	4	-12	32.004	31.356
-11	3	11	44.585	43.949	-6	4	-12	112.110	106.742
-9	3	11	19.707	13.685	-4	4	-12	225.301	220.276
-7	3	11	12.447	9.503	-2	4	-12	38.537	37.819
-5	3	11	44.886	43.669	0	4	-12	40.341	40.018
-3	3	11	34.256	30.195	2	4	-12	39.443	38.802
1	3	11	37.963	35.978	4	4	-12	61.220	60.999
3	3	11	53.654	55.232	6	4	-12	21.329	18.283

Santaclarita Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
8	4	-12	22.411	22.619	6	4	-8	51.150	51.046
10	4	-12	37.447	36.028	8	4	-8	128.110	128.831
14	4	-12	37.394	36.218	10	4	-8	36.923	37.835
-17	4	-11	94.955	99.210	12	4	-8	16.463	17.254
-13	4	-11	44.951	42.161	14	4	-8	29.719	27.585
-11	4	-11	29.516	32.277	-19	4	-7	61.593	59.888
-5	4	-11	46.480	45.931	-17	4	-7	16.752	16.263
-3	4	-11	52.089	53.732	-15	4	-7	52.138	51.343
1	4	-11	38.996	35.629	-21	0	1	97.894	92.780
3	4	-11	149.240	146.547	-19	0	1	73.858	72.044
5	4	-11	171.622	169.036	-13	4	-7	16.906	21.497
7	4	-11	15.805	10.413	-11	4	-7	10.378	1.483
9	4	-11	21.081	22.648	-7	4	-7	28.691	26.405
11	4	-11	14.016	14.930	-5	4	-7	18.459	20.651
13	4	-11	24.435	17.415	-3	4	-7	38.776	40.905
15	4	-11	14.110	11.339	-1	4	-7	24.024	27.126
-18	4	-10	78.325	74.600	3	4	-7	11.850	10.478
-16	4	-10	93.886	90.628	5	4	-7	70.301	70.158
-14	4	-10	21.976	20.312	7	4	-7	131.167	127.394
-12	4	-10	45.988	48.967	9	4	-7	261.549	260.413
-10	4	-10	25.801	25.388	11	4	-7	23.813	21.119
-8	4	-10	113.061	115.667	13	4	-7	52.179	50.032
-6	4	-10	68.858	68.049	17	4	-7	58.740	56.585
-2	4	-10	22.549	21.094	-20	4	-6	14.467	9.908
0	4	-10	17.504	19.664	-18	4	-6	28.996	25.846
2	4	-10	32.045	29.562	-16	4	-6	38.541	36.203
4	4	-10	38.935	40.859	-14	4	-6	155.659	149.897
6	4	-10	15.000	16.873	-12	4	-6	219.817	213.010
10	4	-10	126.646	123.627	-10	4	-6	48.715	49.456
12	4	-10	84.061	82.698	-8	4	-6	73.427	74.379
14	4	-10	33.959	31.848	-4	4	-6	45.919	49.709
-17	4	-9	74.077	71.074	-2	4	-6	112.821	113.670
-15	4	-9	16.923	2.768	0	4	-6	16.049	14.997
-13	4	-9	111.280	110.237	2	4	-6	10.045	12.239
-11	4	-9	48.362	45.194	4	4	-6	9.159	3.470
-9	4	-9	136.191	135.036	6	4	-6	25.577	25.630
-7	4	-9	103.927	100.256	8	4	-6	66.878	67.584
-5	4	-9	33.581	30.407	10	4	-6	26.955	23.254
-3	4	-9	48.207	48.072	12	4	-6	22.927	23.610
-1	4	-9	67.427	67.823	14	4	-6	35.959	36.264
1	4	-9	136.130	141.553	16	4	-6	97.606	97.452
3	4	-9	22.329	22.037	18	4	-6	112.073	108.571
5	4	-9	82.675	83.344	-19	4	-5	44.280	46.284
9	4	-9	51.541	49.917	-17	4	-5	22.000	21.330
-18	4	-8	41.028	37.699	-15	4	-5	25.000	24.713
-16	4	-8	33.325	36.912	-13	4	-5	31.760	30.153
-8	4	-8	39.085	36.964	-11	4	-5	25.813	22.902
-6	4	-8	11.720	13.971	-9	4	-5	163.394	162.694
-4	4	-8	145.431	144.433	-7	4	-5	228.504	224.250
-2	4	-8	96.293	95.416	-5	4	-5	406.524	402.199
0	4	-8	238.557	235.800	-3	4	-5	144.809	146.859
2	4	-8	33.866	32.937	-1	4	-5	13.663	10.667
4	4	-8	59.841	59.170	1	4	-5	62.801	66.450

Santaclarita Structure Factor Table (based on I:-ceII)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	4	-5	124.715	127.548	6	4	-2	30.797	30.371
5	4	-5	84.130	87.302	8	4	-2	22.910	25.286
7	4	-5	62.833	64.610	10	4	-2	52.959	52.688
9	4	-5	62.626	62.452	12	4	-2	88.540	90.304
15	4	-5	27.183	28.124	16	4	-2	70.089	68.947
17	4	-5	49.488	50.307	18	4	-2	22.789	21.085
-20	4	-4	20.439	20.398	-21	4	-1	49.825	51.639
-18	4	-4	76.455	73.448	-19	4	-1	16.037	17.091
-16	4	-4	17.516	13.813	-17	4	-1	34.797	31.916
-14	4	-4	42.626	40.939	-15	4	-1	25.358	25.989
-12	4	-4	19.333	21.376	-13	4	-1	16.122	14.505
-10	4	-4	82.317	80.363	-11	4	-1	18.484	21.049
-8	4	-4	11.236	11.683	-9	4	-1	13.606	9.659
-6	4	-4	30.000	32.624	-7	4	-1	73.923	75.567
-4	4	-4	42.427	43.336	-5	4	-1	25.362	24.397
-2	4	-4	29.423	31.090	-3	4	-1	157.488	158.115
0	4	-4	103.329	105.163	-1	4	-1	196.419	192.808
2	4	-4	228.159	232.069	1	4	-1	200.659	202.457
4	4	-4	275.663	277.600	3	4	-1	39.264	35.327
8	4	-4	57.423	57.220	5	4	-1	38.272	39.774
12	4	-4	91.427	90.739	7	4	-1	147.707	153.856
14	4	-4	28.134	6.482	9	4	-1	75.687	76.173
16	4	-4	48.106	48.831	11	4	-1	15.797	12.489
18	4	-4	14.386	12.607	13	4	-1	31.341	27.706
-21	4	-3	40.715	43.502	15	4	-1	21.089	15.412
-19	4	-3	26.390	11.807	-21	4	1	41.102	41.534
-17	4	-3	144.463	139.331	-19	4	1	15.911	14.935
-15	4	-3	49.866	46.374	-17	4	1	87.163	84.801
-11	4	-3	16.260	14.085	-15	4	1	17.923	17.894
-9	4	-3	74.833	76.609	-13	4	1	291.398	288.592
-7	4	-3	80.744	79.378	-11	4	1	70.073	68.382
-5	4	-3	93.939	89.902	-9	4	1	16.951	15.089
-3	4	-3	35.463	33.627	-7	4	1	62.955	64.980
-1	4	-3	110.898	110.801	-5	4	1	78.195	81.092
1	4	-3	42.333	42.620	-3	4	1	87.963	87.699
3	4	-3	123.183	130.105	-1	4	1	119.354	118.384
5	4	-3	14.134	16.668	1	4	1	17.760	16.022
7	4	-3	16.533	19.850	3	4	1	25.902	21.063
11	4	-3	120.898	120.682	5	4	1	94.219	95.098
13	4	-3	143.886	143.792	7	4	1	79.447	85.181
-20	4	-2	31.724	33.275	9	4	1	42.459	41.735
15	4	-3	81.711	82.302	11	4	1	34.232	38.279
17	4	-3	42.630	42.197	13	4	1	39.492	33.528
-14	4	-2	13.130	12.223	15	4	1	72.886	115.541
-12	4	-2	48.585	50.347	17	4	1	91.894	89.470
-10	4	-2	99.041	99.292	-20	4	2	24.435	22.717
-8	4	-2	255.431	253.725	-18	4	2	52.687	52.521
-6	4	-2	64.350	64.012	-16	4	2	13.878	11.847
-4	4	-2	80.496	82.343	-14	4	2	12.593	2.407
-2	4	-2	69.484	73.301	-12	4	2	26.992	28.005
0	4	-2	121.667	121.895	-8	4	2	55.431	54.588
2	4	-2	34.301	35.112	-6	4	2	14.000	11.446
4	4	-2	104.911	101.230	-4	4	2	246.553	249.272

Santaclaraite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	4	2	126.675	131.822	9	4	5	48.972	46.455
0	4	2	55.276	58.167	11	4	5	37.106	33.301
2	4	2	70.606	74.218	13	4	5	48.772	52.628
4	4	2	66.902	67.332	15	4	5	19.541	18.453
6	4	2	43.667	23.141	-18	4	6	23.650	25.039
8	4	2	55.024	55.027	-14	4	6	102.423	103.146
10	4	2	11.817	6.824	-12	4	6	25.813	26.416
12	4	2	15.159	11.606	-10	4	6	66.614	69.123
14	4	2	92.264	90.609	-8	4	6	53.882	56.717
16	4	2	57.894	61.087	-6	4	6	15.573	12.806
-19	4	3	16.354	15.537	-4	4	6	77.496	76.240
-13	4	3	31.337	32.704	-2	4	6	90.077	89.133
-11	4	3	25.947	25.982	0	4	6	320.171	321.042
-9	4	3	13.313	10.222	2	4	6	57.106	58.229
-7	4	3	44.240	47.471	4	4	6	54.122	53.874
-5	4	3	9.764	12.683	6	4	6	28.203	30.604
-3	4	3	30.293	31.900	8	4	6	72.333	72.573
-1	4	3	29.130	28.271	10	4	6	75.427	73.821
1	4	3	98.756	98.140	12	4	6	37.041	35.984
3	4	3	56.609	54.725	-17	4	7	63.402	63.977
5	4	3	102.114	104.464	-15	4	7	45.512	47.351
7	4	3	59.008	61.723	-13	4	7	99.626	99.656
9	4	3	32.350	33.766	-11	4	7	23.033	23.014
11	4	3	104.695	107.741	-5	4	7	118.122	120.517
15	4	3	57.569	58.833	-3	4	7	33.610	34.587
17	4	3	34.724	35.668	-1	4	7	94.000	98.284
-18	4	4	124.646	116.871	1	4	7	54.951	56.883
-16	4	4	85.098	79.133	3	4	7	45.841	45.163
-14	4	4	73.122	75.484	5	4	7	48.354	51.370
-12	4	4	27.041	25.440	7	4	7	40.805	40.693
-10	4	4	31.626	32.520	9	4	7	136.736	128.862
-6	4	4	24.382	22.212	11	4	7	33.159	36.026
-4	4	4	27.305	24.099	13	4	7	29.671	30.470
-2	4	4	9.915	11.435	-16	4	8	37.976	36.989
0	4	4	9.776	12.452	-14	4	8	62.028	59.881
2	4	4	44.402	45.314	-12	4	8	50.276	51.336
4	4	4	66.976	73.844	-10	4	8	15.512	12.816
6	4	4	9.549	5.512	-8	4	8	31.923	32.241
8	4	4	28.805	26.207	-6	4	8	65.492	65.883
10	4	4	57.634	58.691	-4	4	8	99.110	95.759
12	4	4	16.049	19.394	0	4	8	20.581	16.989
14	4	4	58.093	60.217	2	4	8	32.159	33.347
16	4	4	36.500	34.452	4	4	8	46.480	50.359
-13	4	5	108.053	111.585	6	4	8	31.817	30.855
-11	4	5	23.122	16.112	8	4	8	94.951	99.990
-9	4	5	279.207	280.591	10	4	8	18.825	16.668
-7	4	5	97.606	97.214	-15	4	9	24.675	18.894
-3	4	5	22.780	22.296	-13	4	9	21.984	21.655
-1	4	5	121.594	123.570	-9	4	9	11.858	16.071
1	4	5	85.833	84.615	-7	4	9	17.256	17.612
3	4	5	26.423	24.681	-5	4	9	112.817	112.397
5	4	5	77.382	74.655	3	4	9	87.089	88.194
7	4	5	75.016	74.852	5	4	9	95.915	95.960

Santaclarite Structure Factor Table (based on J=cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
7	4	9	66.732	66.696	-1	5	-13	57.195	56.574
9	4	9	62.776	63.052	1	5	-13	23.427	21.627
11	4	9	23.130	19.289	7	5	-13	32.459	30.191
-12	4	10	49.260	47.244	9	5	-13	22.646	19.611
-10	4	10	74.610	74.817	-14	5	-12	25.902	21.234
-8	4	10	49.467	46.232	-10	5	-12	22.171	20.587
-6	4	10	36.321	35.092	-8	5	-12	27.667	24.606
-4	4	10	22.484	24.027	-4	5	-12	182.533	177.009
0	4	10	33.065	33.517	-2	5	-12	163.033	163.218
2	4	10	22.846	23.450	2	5	-12	29.573	24.725
4	4	10	110.146	111.806	4	5	-12	35.028	32.970
6	4	10	17.724	14.648	6	5	-12	72.179	70.585
8	4	10	12.650	10.140	8	5	-12	43.789	41.655
-11	4	11	42.663	43.379	10	5	-12	43.846	41.999
-9	4	11	99.585	97.704	-15	5	-11	33.581	30.830
-7	4	11	33.805	34.218	-13	5	-11	55.390	54.832
-5	4	11	57.402	57.205	-11	5	-11	20.000	23.408
-3	4	11	14.195	10.356	-9	5	-11	14.809	15.119
-1	4	11	53.606	53.421	-5	5	-11	26.516	25.427
1	4	11	59.268	56.123	-1	5	-11	22.902	22.895
3	4	11	86.516	88.855	1	5	-11	42.346	39.979
-6	4	12	66.748	68.211	3	5	-11	73.992	74.140
-4	4	12	22.650	25.211	5	5	-11	205.423	201.196
-2	4	12	104.520	103.663	7	5	-11	43.244	39.380
0	4	12	94.671	94.122	9	5	-11	59.130	57.404
2	4	12	17.980	18.304	11	5	-11	47.268	45.857
-6	5	-16	74.728	73.009	13	5	-11	76.024	75.341
-4	5	-16	15.341	12.449	-16	5	-10	63.114	61.366
0	5	-16	52.317	52.489	-14	5	-10	82.374	76.902
2	5	-16	68.423	65.749	-12	5	-10	35.675	34.925
-9	5	-15	14.167	16.845	-10	5	-10	28.768	26.731
-7	5	-15	48.276	46.801	-8	5	-10	50.500	50.130
-3	5	-15	69.951	69.513	-6	5	-10	76.504	75.285
-1	5	-15	13.195	9.737	-4	5	-10	97.585	97.725
1	5	-15	130.089	127.079	-2	5	-10	63.967	64.814
3	5	-15	105.524	102.287	0	5	-10	42.882	42.170
5	5	-15	53.472	52.475	4	5	-10	66.163	66.559
-12	5	-14	35.370	33.000	6	5	-10	46.593	45.913
-10	5	-14	20.004	11.784	8	5	-10	33.028	32.993
-8	5	-14	35.817	36.813	10	5	-10	17.362	19.937
-6	5	-14	38.557	37.042	12	5	-10	44.687	41.613
-2	5	-14	30.931	28.265	14	5	-10	137.126	134.726
0	5	-14	27.236	27.333	-17	5	-9	25.797	27.188
2	5	-14	52.130	52.890	-15	5	-9	17.663	16.172
6	5	-14	41.488	40.643	-13	5	-9	40.724	41.921
8	5	-14	34.683	30.301	-9	5	-9	23.748	25.646
10	5	-14	139.646	136.319	-7	5	-9	143.443	138.242
-13	5	-13	72.833	71.201	-5	5	-9	112.402	112.016
-11	5	-13	168.711	165.881	-3	5	-9	20.280	17.798
-9	5	-13	76.561	74.030	-1	5	-9	67.329	67.415
-7	5	-13	34.691	33.200	1	5	-9	99.980	101.042
-5	5	-13	34.585	33.275	3	5	-9	107.516	107.883
-3	5	-13	73.492	73.138	5	5	-9	98.061	95.881

Santaclaraite Structure Factor Table (based on JI-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
9	5	-9	16.906	12.547	-15	5	-5	12.833	14.666
11	5	-9	16.671	17.568	-13	5	-5	10.354	11.420
13	5	-9	62.122	58.348	-11	5	-5	34.764	32.155
15	5	-9	25.618	22.255	-9	5	-5	46.081	49.485
-18	5	-8	74.000	76.526	-7	5	-5	67.175	63.708
-16	5	-8	32.850	33.998	-5	5	-5	86.488	84.078
-14	5	-8	56.480	55.699	-3	5	-5	197.707	197.045
-12	5	-8	27.081	26.669	-1	5	-5	182.866	187.431
-10	5	-8	16.236	18.230	1	5	-5	38.337	35.587
-8	5	-8	13.297	14.289	5	5	-5	34.992	34.338
-6	5	-8	27.260	12.353	7	5	-5	85.171	86.508
-2	5	-8	53.528	53.251	9	5	-5	142.012	140.595
0	5	-8	75.305	72.524	13	5	-5	51.224	50.033
2	5	-8	231.197	225.142	15	5	-5	24.463	23.060
4	5	-8	63.882	67.170	17	5	-5	83.232	81.020
6	5	-8	53.398	53.322	-20	5	-4	24.646	24.218
8	5	-8	45.780	45.457	-18	5	-4	27.760	29.044
10	5	-8	30.984	29.326	-16	5	-4	67.321	70.235
12	5	-8	45.406	44.689	-14	5	-4	28.411	29.876
16	5	-8	13.492	10.852	-12	5	-4	44.772	42.692
-19	5	-7	116.102	109.369	-6	5	-4	32.923	36.633
-17	5	-7	53.919	53.182	-4	5	-4	24.272	23.189
-13	5	-7	65.110	64.761	-2	5	-4	12.894	14.175
-11	5	-7	22.175	23.307	0	5	-4	74.866	76.538
-9	5	-7	89.016	89.973	2	5	-4	87.211	90.300
-7	5	-7	9.764	8.393	4	5	-4	38.817	37.499
-5	5	-7	19.415	17.804	6	5	-4	86.943	87.136
-3	5	-7	49.492	49.325	8	5	-4	119.419	123.081
-1	5	-7	20.293	13.805	10	5	-4	72.935	75.256
1	5	-7	10.602	9.443	12	5	-4	35.016	36.154
5	5	-7	18.541	20.286	14	5	-4	24.528	22.785
7	5	-7	76.268	77.765	16	5	-4	25.329	22.402
9	5	-7	157.874	154.097	-19	5	-3	43.024	40.317
11	5	-7	96.057	92.857	-17	5	-3	35.906	31.771
13	5	-7	14.138	16.578	-15	5	-3	156.293	151.578
15	5	-7	30.423	31.302	-13	5	-3	126.947	123.918
-20	5	-6	58.691	56.109	-11	5	-3	38.484	38.946
-18	5	-6	54.240	50.661	-9	5	-3	46.455	48.556
-16	5	-6	89.236	87.125	-7	5	-3	12.764	14.499
-14	5	-6	53.191	52.814	-3	5	-3	43.263	44.027
-12	5	-6	229.415	224.998	-1	5	-3	40.187	39.619
-10	5	-6	145.317	139.688	1	5	-3	56.394	56.276
-8	5	-6	62.626	65.262	3	5	-3	53.325	54.074
-6	5	-6	25.797	25.662	5	5	-3	14.553	11.404
-4	5	-6	53.236	55.845	7	5	-3	46.106	48.723
-2	5	-6	12.467	13.378	9	5	-3	29.512	31.846
0	5	-6	86.118	86.192	11	5	-3	40.917	57.899
2	5	-6	44.398	45.824	15	5	-3	82.463	83.774
4	5	-6	19.496	19.073	17	5	-3	59.959	60.532
6	5	-6	16.528	15.045	-20	5	-2	52.374	53.802
8	5	-6	91.508	92.688	-18	5	-2	16.285	12.053
10	5	-6	20.947	20.690	-16	5	-2	11.195	10.098
16	5	-6	61.041	62.097	-14	5	-2	10.659	11.436

Santaclaraite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-12	5	-2	103.459	106.652	2	5	2	29.398	27.536
-10	5	-2	44.020	43.157	4	5	2	52.134	53.106
-8	5	-2	333.918	329.954	6	5	2	143.020	147.350
-6	5	-2	231.224	226.752	8	5	2	23.642	22.628
-4	5	-2	50.232	51.690	10	5	2	61.451	61.037
-2	5	-2	57.341	58.584	12	5	2	41.085	40.815
0	5	-2	34.337	37.143	14	5	2	40.199	36.295
2	5	-2	119.520	124.393	-17	5	3	18.776	17.938
6	5	-2	13.577	17.426	-15	5	3	70.211	69.259
10	5	-2	37.870	36.223	-13	5	3	10.787	10.390
14	5	-2	19.996	20.915	-11	5	3	45.679	44.348
16	5	-2	42.041	40.180	-9	5	3	68.724	68.335
-19	5	-1	58.293	52.764	-5	5	3	63.785	64.151
-17	5	-1	15.252	13.124	-3	5	3	61.439	64.852
-15	5	-1	15.195	1.952	-1	5	3	17.264	20.303
-13	5	-1	45.008	44.140	1	5	3	21.902	19.343
-11	5	-1	98.911	101.747	3	5	3	28.841	27.435
-9	5	-1	63.411	64.521	5	5	3	178.634	181.722
-7	5	-1	36.602	40.477	7	5	3	46.163	49.310
-3	5	-1	94.955	96.042	9	5	3	36.463	37.974
-1	5	-1	54.268	50.769	11	5	3	14.272	15.093
1	5	-1	453.764	461.477	13	5	3	60.805	63.667
3	5	-1	215.659	220.884	15	5	3	113.154	114.559
5	5	-1	39.037	40.569	-18	5	4	73.846	74.244
7	5	-1	45.744	47.125	-16	5	4	87.398	86.856
9	5	-1	63.297	63.943	-14	5	4	189.882	190.075
11	5	-1	96.032	95.138	-12	5	4	12.244	15.195
13	5	-1	30.573	27.024	-10	5	4	14.354	13.599
17	5	-1	45.634	45.178	-8	5	4	118.114	121.314
-19	5	1	12.248	4.922	-6	5	4	87.419	88.540
-17	5	1	40.341	35.744	-4	5	4	30.069	33.685
-13	5	1	60.463	58.656	-2	5	4	73.167	73.028
-11	5	1	44.715	42.220	0	5	4	13.870	12.887
-9	5	1	145.785	149.376	2	5	4	18.841	16.597
-7	5	1	77.776	78.161	4	5	4	107.415	110.376
-5	5	1	14.984	14.609	6	5	4	59.435	64.112
-3	5	1	120.939	123.239	8	5	4	11.561	8.077
1	5	1	35.541	38.345	10	5	4	32.350	35.852
3	5	1	71.008	68.715	12	5	4	36.821	32.815
5	5	1	53.807	56.518	14	5	4	99.581	99.426
7	5	1	19.638	17.059	-15	5	5	22.085	24.633
9	5	1	76.817	79.882	-13	5	5	17.419	14.495
11	5	1	78.606	82.181	-11	5	5	12.533	14.082
15	5	1	66.508	67.932	-9	5	5	20.565	16.625
-18	5	2	44.004	43.209	-7	5	5	115.102	112.618
-16	5	2	16.955	17.568	-5	5	5	190.675	194.377
-14	5	2	17.695	19.282	-3	5	5	47.394	46.787
-12	5	2	26.443	29.943	-1	5	5	47.736	50.776
-10	5	2	25.301	24.855	1	5	5	124.679	127.316
-8	5	2	27.488	27.851	3	5	5	61.289	60.986
-4	5	2	119.642	120.337	5	5	5	56.805	58.570
-2	5	2	12.687	8.513	9	5	5	20.785	23.316
0	5	2	27.878	31.927	11	5	5	51.902	51.462

Santaclaraite Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
13	5	5	123.480	124.698	-2	6	-16	19.211	21.732
-16	5	6	20.736	24.605	0	6	-16	51.752	50.078
-14	5	6	28.882	29.260	-7	6	-15	44.122	41.806
-10	5	6	37.573	38.919	-5	6	-15	35.728	37.883
-8	5	6	15.398	15.545	-3	6	-15	52.837	54.938
-6	5	6	35.923	36.845	1	6	-15	17.626	19.836
-4	5	6	40.706	42.166	3	6	-15	98.309	96.234
-2	5	6	26.325	30.708	5	6	-15	110.305	108.999
0	5	6	42.528	43.418	-10	6	-14	26.236	26.289
2	5	6	41.049	42.707	-8	6	-14	94.382	92.340
4	5	6	101.167	102.312	-6	6	-14	29.390	28.754
6	5	6	12.650	11.231	-4	6	-14	17.276	16.504
8	5	6	74.313	76.911	-2	6	-14	52.297	50.099
10	5	6	80.886	83.010	6	6	-14	22.321	17.139
12	5	6	42.102	44.046	8	6	-14	28.972	29.236
-15	5	7	25.927	29.055	-13	6	-13	77.793	78.093
-13	5	7	20.118	18.976	-11	6	-13	66.492	64.955
-11	5	7	72.874	68.856	-9	6	-13	143.354	138.530
-9	5	7	36.520	33.654	-7	6	-13	67.980	65.038
-7	5	7	46.252	44.064	-3	6	-13	12.898	14.236
-5	5	7	40.228	38.218	-1	6	-13	32.866	17.858
-3	5	7	42.350	38.229	1	6	-13	92.890	91.772
0	5	7	47.350	47.037	3	6	-13	28.012	28.292
-14	5	8	96.866	96.909	5	6	-13	42.402	41.945
-12	5	8	39.577	38.506	9	6	-13	48.841	47.898
-10	5	8	140.699	139.306	-14	6	-12	12.817	14.300
-4	5	8	27.516	27.500	-12	6	-12	37.923	37.734
-2	5	8	71.520	70.082	-10	6	-12	59.020	56.049
2	5	8	46.724	45.870	-6	6	-12	17.618	15.059
4	5	8	18.846	23.269	-4	6	-12	55.382	53.122
6	5	8	57.817	54.479	-2	6	-12	79.919	77.962
10	5	8	15.378	12.037	0	6	-12	129.646	127.079
-13	5	9	30.191	28.638	2	6	-12	33.679	33.496
-11	5	9	27.260	26.900	4	6	-12	50.967	48.718
-9	5	9	28.126	28.128	8	6	-12	88.008	84.889
-7	5	9	19.488	21.088	10	6	-12	77.642	75.425
-5	5	9	52.996	54.249	-15	6	-11	73.467	75.890
-3	5	9	47.191	48.803	-11	6	-11	33.195	32.512
1	5	9	134.593	132.489	-7	6	-11	21.793	20.784
5	5	9	12.358	7.569	-5	6	-11	12.858	13.193
7	5	9	64.085	63.315	-3	6	-11	19.081	16.145
10	5	9	52.077	52.832	5	6	-11	31.972	31.721
-6	5	10	82.817	83.291	7	6	-11	68.110	66.371
-4	5	10	60.813	62.257	9	6	-11	116.959	113.826
-2	5	10	77.248	78.424	-14	6	-10	119.175	116.666
0	5	10	26.321	27.867	-12	6	-10	130.988	128.637
2	5	10	25.195	24.487	-4	6	-10	19.642	18.561
4	5	10	33.817	35.665	-2	6	-10	53.878	54.348
-5	5	11	59.732	55.546	2	6	-10	29.585	30.649
-3	5	11	45.134	42.717	4	6	-10	13.236	11.823
-1	5	11	31.346	29.932	6	6	-10	30.780	31.544
1	5	11	43.602	40.848	8	6	-10	46.585	43.525
-4	6	-16	106.224	102.440	10	6	-10	22.785	21.672



Santaclarita Structure Factor Table (based on R-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
12	6	-10	31.512	32.155	4	6	-6	76.886	75.363
-15	6	-9	17.244	15.771	8	6	-6	33.955	33.718
-11	6	-9	38.606	29.149	10	6	-6	52.882	52.375
-9	6	-9	71.297	70.423	12	6	-6	90.776	91.394
-7	6	-9	126.634	124.907	14	6	-6	13.809	14.859
-5	6	-9	272.675	265.795	-15	6	-5	28.476	25.770
-3	6	-9	120.248	120.101	-11	6	-5	31.211	31.782
-1	6	-9	56.435	57.204	-9	6	-5	20.333	22.063
3	6	-9	26.829	24.250	-7	6	-5	48.504	49.709
5	6	-9	13.598	13.189	-5	6	-5	14.899	16.276
7	6	-9	86.232	87.295	-3	6	-5	100.711	103.304
9	6	-9	21.012	14.689	-1	6	-5	18.923	15.128
11	6	-9	34.394	32.481	1	6	-5	101.915	100.239
-18	6	-8	68.370	65.206	3	6	-5	59.346	60.026
-16	6	-8	30.451	30.479	7	6	-5	89.150	92.574
-14	6	-8	37.459	37.416	9	6	-5	41.833	42.202
-12	6	-8	32.224	31.478	11	6	-5	13.707	17.018
-10	6	-8	74.988	73.593	13	6	-5	52.760	51.384
-6	6	-8	33.037	35.652	-16	6	-4	15.752	14.232
-2	6	-8	61.297	60.411	-14	6	-4	100.622	100.354
0	6	-8	57.902	57.746	-12	6	-4	54.789	59.501
2	6	-8	237.939	235.387	-10	6	-4	43.520	40.247
4	6	-8	233.561	233.184	-8	6	-4	16.605	15.003
6	6	-8	43.837	43.974	-6	6	-4	17.081	17.639
8	6	-8	83.443	81.343	-4	6	-4	37.102	38.106
10	6	-8	28.455	28.717	-2	6	-4	51.858	53.186
12	6	-8	80.939	78.373	2	6	-4	18.362	17.943
14	6	-8	36.175	33.969	4	6	-4	51.618	51.401
-19	6	-7	41.537	39.066	6	6	-4	138.065	143.256
-17	6	-7	130.760	125.781	8	6	-4	113.549	118.160
-15	6	-7	51.589	47.831	12	6	-4	28.337	26.747
-13	6	-7	19.037	19.294	-19	6	-3	45.179	45.293
-11	6	-7	30.024	27.937	-17	6	-3	78.931	77.702
-9	6	-7	60.837	59.164	-15	6	-3	45.963	44.153
-7	6	-7	78.207	78.132	-13	6	-3	237.886	231.084
-5	6	-7	52.297	51.992	-11	6	-3	85.634	84.565
-1	6	-7	84.362	86.272	-9	6	-3	13.833	10.790
1	6	-7	59.455	59.950	-5	6	-3	168.504	170.891
3	6	-7	99.825	101.129	-3	6	-3	15.528	15.554
9	6	-7	16.613	14.847	-1	6	-3	70.126	69.332
11	6	-7	149.789	147.984	3	6	-3	17.443	20.227
13	6	-7	106.268	105.010	5	6	-3	101.654	103.212
15	6	-7	34.374	32.325	7	6	-3	69.553	72.499
-16	6	-6	21.874	21.752	11	6	-3	31.850	35.644
-14	6	-6	22.707	20.924	13	6	-3	34.472	30.227
-12	6	-6	14.138	10.251	15	6	-3	88.614	89.933
-10	6	-6	29.138	25.508	-18	6	-2	25.366	24.786
-8	6	-6	156.955	155.302	-16	6	-2	13.317	18.241
-6	6	-6	25.037	28.507	-12	6	-2	15.134	14.498
-4	6	-6	14.138	13.213	-10	6	-2	31.516	24.334
-2	6	-6	31.333	29.482	-8	6	-2	81.768	81.598
0	6	-6	68.797	68.172	-6	6	-2	146.102	141.691
2	6	-6	27.541	28.630	-4	6	-2	299.073	304.978

Santa Clara Site Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	6	-2	83.801	26.749	-9	6	3	28.313	30.994
0	6	-2	7.524	9.915	-7	6	3	32.240	32.028
2	6	-2	74.988	77.204	-5	6	3	98.443	101.803
4	6	-2	75.219	77.114	-1	6	3	120.492	127.431
6	6	-2	9.813	9.456	1	6	3	78.301	81.121
8	6	-2	56.280	54.037	3	6	3	15.301	22.562
10	6	-2	35.102	32.714	7	6	3	31.159	34.406
12	6	-2	13.768	15.293	9	6	3	186.415	188.386
14	6	-2	82.374	81.187	11	6	3	14.907	8.647
-19	6	-1	36.041	32.368	13	6	3	27.630	27.080
-9	6	-1	21.411	22.314	-16	6	4	88.138	86.149
-7	6	-1	25.110	26.824	-14	6	4	90.947	90.063
-5	6	-1	74.711	76.503	-12	6	4	95.118	96.033
-3	6	-1	29.244	29.748	-10	6	4	31.955	32.648
-1	6	-1	27.029	27.593	-8	6	4	58.346	58.894
1	6	-1	59.833	62.265	-6	6	4	97.927	99.698
5	6	-1	137.581	140.559	-4	6	4	128.431	128.873
7	6	-1	36.126	38.604	-2	6	4	19.073	17.338
11	6	-1	83.752	85.708	0	6	4	30.341	29.678
15	6	-1	45.972	47.060	2	6	4	12.159	10.012
-15	6	1	20.175	18.793	4	6	4	23.118	26.605
-13	6	1	115.394	112.075	6	6	4	44.000	45.415
-11	6	1	22.248	20.320	8	6	4	86.967	89.645
-9	6	1	187.049	184.861	10	6	4	59.955	61.043
-7	6	1	59.037	57.092	-11	6	5	34.711	34.242
-5	6	1	21.772	21.661	-9	6	5	56.069	54.946
-3	6	1	36.098	37.505	-7	6	5	70.427	70.711
-1	6	1	117.650	120.288	-5	6	5	114.110	114.525
1	6	1	29.866	29.718	-3	6	5	23.886	27.141
3	6	1	72.439	71.378	1	6	5	10.703	10.599
5	6	1	12.919	13.360	3	6	5	98.963	101.669
7	6	1	27.683	24.507	5	6	5	65.781	65.459
9	6	1	37.077	33.429	7	6	5	66.150	64.515
11	6	1	15.736	13.573	9	6	5	30.671	28.564
13	6	1	13.276	12.513	11	6	5	23.378	21.839
-18	6	2	15.061	16.515	-12	6	6	76.626	72.336
-16	6	2	12.232	14.883	-10	6	6	47.740	48.313
-14	6	2	53.679	55.688	-8	6	6	37.736	37.067
-12	6	2	12.776	12.946	-6	6	6	24.809	31.581
-10	6	2	36.756	38.168	-4	6	6	16.809	18.681
-8	6	2	46.142	45.948	-2	6	6	17.602	11.433
-4	6	2	64.484	64.430	2	6	6	19.045	17.576
-2	6	2	32.041	30.756	4	6	6	78.093	81.940
0	6	2	291.573	293.338	6	6	6	22.378	15.026
4	6	2	49.472	48.662	10	6	6	15.837	17.099
6	6	2	41.585	44.189	-13	6	7	30.309	29.947
8	6	2	79.179	80.691	-11	6	7	56.772	57.138
10	6	2	52.350	53.654	-9	6	7	56.443	55.274
12	6	2	53.008	52.901	-7	6	7	37.821	35.055
-17	6	3	26.675	26.432	-5	6	7	12.488	15.783
-15	6	3	51.906	51.765	-3	6	7	67.671	67.904
-13	6	3	44.370	41.079	-1	6	7	34.142	35.299
-11	6	3	53.638	52.521	1	6	7	38.882	38.189

Santaclarite Structure Factor Table (based on J-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	6	7	59.154	63.608	-13	7	-11	107.106	106.320
5	6	7	16.776	28.028	-11	7	-11	57.732	61.073
7	6	7	51.260	52.286	-9	7	-11	60.577	60.753
-12	6	8	15.370	10.585	-7	7	-11	33.699	22.243
-8	6	8	56.898	59.800	-5	7	-11	27.317	26.085
-6	6	8	68.138	70.314	-3	7	-11	35.228	35.704
-4	6	8	45.699	44.874	1	7	-11	32.415	31.134
-2	6	8	107.264	109.290	7	7	-11	48.703	47.092
0	6	8	107.833	110.330	9	7	-11	80.800	78.958
2	6	8	18.313	14.394	-16	7	-10	38.297	37.318
4	6	8	74.874	76.227	-14	7	-10	35.817	33.839
6	6	8	14.443	14.606	-12	7	-10	174.321	167.648
-9	6	9	64.341	64.867	-10	7	-10	164.211	157.945
-7	6	9	17.354	14.738	-6	7	-10	64.561	62.966
-5	6	9	45.699	43.479	-4	7	-10	96.183	96.289
-3	6	9	60.313	60.289	0	7	-10	51.118	48.219
-1	6	9	53.756	53.188	2	7	-10	11.199	10.651
1	6	9	24.455	28.594	4	7	-10	26.959	0.641
3	6	9	32.711	35.349	6	7	-10	38.024	38.783
-7	7	-15	13.683	5.501	8	7	-10	55.744	53.889
-5	7	-15	14.382	12.582	-15	7	-9	34.801	36.603
-3	7	-15	12.955	12.320	-13	7	-9	28.455	24.873
-1	7	-15	18.581	17.779	-11	7	-9	39.159	28.851
3	7	-15	49.057	48.220	-9	7	-9	23.028	25.834
-10	7	-14	52.492	49.423	-7	7	-9	55.346	54.173
-8	7	-14	38.093	36.792	-5	7	-9	24.553	21.802
-6	7	-14	39.756	40.944	-3	7	-9	203.394	200.565
-4	7	-14	43.675	42.420	-1	7	-9	132.220	131.118
-2	7	-14	41.439	38.493	1	7	-9	19.435	15.825
0	7	-14	37.321	46.166	5	7	-9	57.268	56.982
2	7	-14	41.557	40.013	9	7	-9	64.073	62.093
4	7	-14	29.252	28.102	11	7	-9	39.602	37.664
6	7	-14	16.504	10.422	-16	7	-8	58.825	58.982
-9	7	-13	16.272	11.836	-14	7	-8	62.504	58.845
-7	7	-13	84.028	79.661	-8	7	-8	21.301	19.893
-5	7	-13	30.756	32.726	-6	7	-8	41.541	42.099
-1	7	-13	24.016	20.678	-4	7	-8	56.333	54.991
1	7	-13	45.118	44.759	-2	7	-8	25.102	24.105
3	7	-13	71.541	69.989	0	7	-8	18.394	19.070
5	7	-13	64.898	65.023	2	7	-8	11.012	9.567
7	7	-13	20.459	16.452	4	7	-8	32.874	33.390
-14	7	-12	18.691	16.574	6	7	-8	101.541	100.205
-12	7	-12	14.492	14.057	8	7	-8	44.923	45.944
-10	7	-12	12.785	13.989	10	7	-8	14.077	8.184
-8	7	-12	43.748	42.260	-17	7	-7	35.053	32.497
-6	7	-12	26.610	26.086	-15	7	-7	92.346	88.273
-4	7	-12	24.793	24.546	-13	7	-7	73.175	71.156
-2	7	-12	23.646	24.293	-9	7	-7	60.008	60.033
0	7	-12	59.618	57.584	-7	7	-7	30.037	29.503
2	7	-12	78.866	76.161	-5	7	-7	23.199	21.475
6	7	-12	30.927	31.598	-3	7	-7	55.435	56.857
8	7	-12	12.321	15.439	-1	7	-7	11.146	10.665
-15	7	-11	18.870	16.134	1	7	-7	20.305	20.575

Santaclaraite Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	7	-7	11.484	9.660	5	7	-3	15.154	15.758
5	7	-7	23.805	22.876	7	7	-3	21.089	16.100
7	7	-7	37.785	43.033	9	7	-3	97.150	100.982
11	7	-7	52.061	52.161	11	7	-3	83.825	84.501
-12	7	-6	56.691	55.256	-18	7	-2	48.748	47.628
-10	7	-6	57.459	53.967	-16	7	-2	35.480	35.824
-8	7	-6	123.154	122.376	-14	7	-2	16.476	20.990
-6	7	-6	164.992	162.035	-12	7	-2	15.650	15.074
-4	7	-6	17.244	19.374	-10	7	-2	14.907	15.055
-2	7	-6	87.232	88.502	-8	7	-2	79.163	77.769
0	7	-6	90.366	92.438	-6	7	-2	55.500	59.883
2	7	-6	66.378	65.971	-4	7	-2	93.959	93.507
4	7	-6	44.679	44.615	-2	7	-2	61.980	61.127
6	7	-6	16.825	15.270	0	7	-2	54.467	58.688
8	7	-6	30.390	29.419	2	7	-2	77.561	78.989
10	7	-6	59.276	60.440	4	7	-2	87.959	90.625
12	7	-6	13.699	3.267	6	7	-2	82.126	83.920
-17	7	-5	35.545	34.900	8	7	-2	35.126	33.442
-11	7	-5	50.919	53.015	10	7	-2	40.358	38.583
-9	7	-5	16.719	16.004	12	7	-2	12.370	16.905
-7	7	-5	35.179	23.768	-17	7	-1	35.963	33.606
-5	7	-5	11.711	7.239	-15	7	-1	88.126	83.725
-3	7	-5	72.045	72.765	-11	7	-1	28.541	29.262
-1	7	-5	27.667	26.471	-9	7	-1	66.130	63.725
1	7	-5	291.996	295.896	-7	7	-1	11.711	10.480
3	7	-5	113.890	111.357	-5	7	-1	40.634	42.065
5	7	-5	20.057	20.596	-3	7	-1	35.793	37.939
7	7	-5	59.862	59.552	-1	7	-1	20.939	14.207
9	7	-5	88.976	90.605	1	7	-1	34.244	34.666
11	7	-5	52.695	52.769	3	7	-1	50.671	50.695
13	7	-5	31.821	31.184	5	7	-1	99.557	103.616
-18	7	-4	111.183	105.350	9	7	-1	24.394	24.620
-14	7	-4	31.732	30.831	13	7	-1	65.382	69.253
-12	7	-4	25.102	23.861	-17	7	1	21.264	24.388
-10	7	-4	101.797	99.900	-15	7	1	29.537	27.394
-8	7	-4	24.813	25.043	-13	7	1	30.577	30.255
-6	7	-4	13.122	9.276	-11	7	1	55.793	54.885
-4	7	-4	28.967	30.318	-9	7	1	11.866	8.894
-2	7	-4	50.167	52.121	-7	7	1	119.385	119.084
0	7	-4	75.337	76.630	-5	7	1	130.829	134.402
2	7	-4	112.894	116.287	-3	7	1	63.569	64.074
4	7	-4	33.980	35.376	-1	7	1	74.602	79.393
10	7	-4	206.573	206.712	1	7	1	93.614	96.188
12	7	-4	60.211	60.563	3	7	1	91.301	92.465
-17	7	-3	56.508	55.188	5	7	1	67.894	65.059
-13	7	-3	120.309	114.215	7	7	1	47.203	46.050
-11	7	-3	129.691	125.230	9	7	1	39.207	37.532
-9	7	-3	87.293	89.127	-16	7	2	21.301	12.872
-7	7	-3	41.541	39.805	-12	7	2	23.329	25.700
-5	7	-3	28.606	29.555	-8	7	2	53.886	56.075
-3	7	-3	54.427	53.205	-6	7	2	28.313	29.013
-1	7	-3	69.634	71.036	-4	7	2	51.923	53.590
1	7	-3	17.959	15.379	-2	7	2	39.378	41.954

Santalaraite Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	7	2	76.480	79.388	0	7	8	31.467	35.094
2	7	2	63.882	63.978	-8	8	-14	36.008	35.420
4	7	2	112.293	114.402	-6	8	-14	29.957	28.961
6	7	2	44.232	44.812	-2	8	-14	26.996	27.303
8	7	2	73.419	73.739	0	8	-14	21.520	8.378
10	7	2	99.967	100.617	2	8	-14	22.154	23.306
-13	7	3	49.199	50.800	-9	8	-13	55.061	52.469
-11	7	3	107.963	104.737	-7	8	-13	56.598	54.066
-9	7	3	22.659	24.040	-5	8	-13	143.305	137.064
-7	7	3	35.211	30.098	-3	8	-13	77.374	74.499
-5	7	3	30.224	32.647	-1	8	-13	85.503	82.401
-3	7	3	50.667	49.117	1	8	-13	31.350	31.431
-1	7	3	37.528	36.318	3	8	-13	37.138	36.161
1	7	3	22.427	24.992	5	8	-13	26.053	23.254
3	7	3	38.037	40.172	-10	8	-12	11.988	12.691
5	7	3	31.732	30.613	-8	8	-12	16.163	14.856
7	7	3	41.878	43.456	-2	8	-12	11.593	14.138
9	7	3	58.679	60.371	0	8	-12	55.728	53.491
-14	7	4	100.898	100.078	2	8	-12	122.089	118.579
-12	7	4	82.610	82.357	4	8	-12	184.329	178.843
-10	7	4	92.378	93.460	6	8	-12	25.089	21.661
-6	7	4	33.276	35.136	-13	8	-11	53.687	54.443
-4	7	4	18.646	19.788	-11	8	-11	38.622	37.138
-2	7	4	71.024	70.504	-9	8	-11	88.354	85.944
0	7	4	13.207	14.013	-5	8	-11	31.919	33.336
2	7	4	42.439	46.200	-3	8	-11	33.854	31.193
4	7	4	38.252	41.218	-1	8	-11	61.866	58.342
6	7	4	72.569	69.609	1	8	-11	35.236	31.867
8	7	4	43.825	43.757	3	8	-11	49.600	44.761
-13	7	5	13.854	10.306	5	8	-11	20.801	18.022
-11	7	5	26.850	21.561	-14	8	-10	25.467	27.891
-7	7	5	16.728	15.316	-12	8	-10	50.528	48.064
-5	7	5	88.008	87.682	-10	8	-10	95.004	91.934
-3	7	5	39.110	44.658	-8	8	-10	108.890	103.853
-1	7	5	91.650	91.839	-6	8	-10	14.114	13.865
1	7	5	16.659	9.536	-4	8	-10	11.756	6.945
3	7	5	33.858	34.584	-2	8	-10	31.077	32.095
5	7	5	56.492	59.685	0	8	-10	60.138	61.580
7	7	5	19.549	17.872	2	8	-10	23.073	23.504
-12	7	6	18.163	17.679	4	8	-10	22.553	21.733
-10	7	6	14.187	13.421	6	8	-10	23.317	21.684
-6	7	6	49.183	51.525	8	8	-10	41.711	39.498
-4	7	6	32.996	34.238	-15	8	-9	19.923	21.854
-2	7	6	47.252	51.250	-9	8	-9	38.130	39.395
4	7	6	17.024	13.587	-7	8	-9	28.626	27.024
6	7	6	28.138	32.129	-3	8	-9	86.602	83.422
-7	7	7	137.402	139.705	-1	8	-9	66.512	63.229
-5	7	7	14.553	12.270	1	8	-9	43.992	42.304
-3	7	7	56.598	55.504	3	8	-9	50.053	46.252
-1	7	7	15.841	16.283	5	8	-9	14.833	16.637
1	7	7	37.211	31.208	7	8	-9	59.248	58.218
3	7	7	20.366	19.180	9	8	-9	29.423	28.588
-6	7	8	81.073	85.886	-16	8	-8	16.878	15.170

Santaclarite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-14	8	-8	91.496	87.122	0	8	-4	43.720	44.312
-12	8	-8	50.764	50.124	2	8	-4	25.358	22.728
-10	8	-8	21.467	21.833	4	8	-4	39.435	38.742
-8	8	-8	25.240	24.250	6	8	-4	49.976	50.368
-6	8	-8	39.240	38.721	8	8	-4	38.951	39.844
-4	8	-8	64.415	65.578	10	8	-4	82.886	87.845
-2	8	-8	10.748	5.634	-17	8	-3	47.423	47.713
0	8	-8	47.142	44.757	-15	8	-3	21.167	14.895
2	8	-8	22.740	26.228	-13	8	-3	114.220	110.278
4	8	-8	16.650	20.409	-11	8	-3	13.004	12.014
6	8	-8	62.037	65.525	-9	8	-3	132.476	129.804
8	8	-8	63.313	63.550	-7	8	-3	61.321	61.143
10	8	-8	14.984	10.842	-5	8	-3	20.976	21.189
-15	8	-7	21.122	18.415	-3	8	-3	21.720	21.667
-13	8	-7	162.980	156.427	-1	8	-3	93.406	93.502
-11	8	-7	38.707	36.492	1	8	-3	27.012	27.344
-9	8	-7	27.943	23.449	3	8	-3	44.886	42.940
-5	8	-7	173.545	172.340	5	8	-3	25.890	26.776
-3	8	-7	38.996	38.396	7	8	-3	37.358	36.385
-1	8	-7	72.016	70.338	9	8	-3	56.870	58.569
3	8	-7	10.732	10.262	11	8	-3	17.268	17.766
5	8	-7	64.061	64.720	-16	8	-2	25.943	23.531
7	8	-7	44.943	43.925	-14	8	-2	39.955	38.610
9	8	-7	27.061	2.193	-12	8	-2	32.195	32.544
11	8	-7	21.963	18.640	-10	8	-2	59.963	61.152
-14	8	-6	24.171	19.289	-6	8	-2	13.813	6.471
-12	8	-6	17.187	16.278	-4	8	-2	65.260	65.624
-10	8	-6	28.220	27.323	0	8	-2	122.866	128.724
-6	8	-6	107.248	106.707	2	8	-2	14.459	11.733
-4	8	-6	168.195	169.226	8	8	-2	82.341	84.816
-2	8	-6	32.996	33.598	10	8	-2	15.573	1.867
0	8	-6	13.943	11.510	-15	8	-1	20.492	20.760
2	8	-6	26.065	23.758	-13	8	-1	21.020	16.399
4	8	-6	116.520	114.994	-11	8	-1	60.760	58.842
8	8	-6	53.776	53.285	-9	8	-1	35.528	36.674
10	8	-6	31.285	27.499	-7	8	-1	17.199	12.729
-17	8	-5	29.106	29.051	-5	8	-1	48.268	50.194
-15	8	-5	22.325	18.904	-1	8	-1	58.118	61.201
-13	8	-5	25.337	25.207	1	8	-1	38.732	39.875
-11	8	-5	11.045	4.602	3	8	-1	21.134	22.227
-5	8	-5	53.630	52.987	5	8	-1	42.988	39.908
-3	8	-5	24.175	23.110	7	8	-1	26.931	32.873
-1	8	-5	24.724	25.234	9	8	-1	132.041	134.387
1	8	-5	39.488	40.603	-15	8	1	25.663	26.793
3	8	-5	88.541	88.198	-13	8	1	21.500	17.796
5	8	-5	123.240	126.026	-11	8	1	40.142	36.086
9	8	-5	29.821	28.586	-9	8	1	92.142	92.271
11	8	-5	64.654	63.721	-7	8	1	134.394	135.249
-16	8	-4	79.484	74.586	-5	8	1	146.524	148.177
-12	8	-4	20.679	21.128	-3	8	1	62.337	64.088
-10	8	-4	67.931	65.475	-1	8	1	18.923	12.677
-8	8	-4	21.443	22.259	1	8	1	23.768	23.143
-4	8	-4	10.492	11.670	3	8	1	130.898	133.660

Santaclarita Structure Factor Table (based on H-CeJ)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
5	8	1	29.537	31.052	-12	9	-10	66.846	62.900
7	8	1	27.780	26.531	-10	9	-10	31.675	33.204
9	8	1	12.350	8.823	-8	9	-10	89.089	87.521
-12	8	2	30.110	27.734	-6	9	-10	90.065	88.552
-10	8	2	64.093	64.558	-4	9	-10	12.846	13.722
-6	8	2	64.289	64.149	-2	9	-10	19.480	16.197
-4	8	2	52.244	54.086	0	9	-10	85.618	85.628
-2	8	2	20.598	20.872	4	9	-10	48.337	45.142
0	8	2	42.963	45.121	-13	9	-9	38.098	35.872
2	8	2	74.276	75.343	-5	9	-9	19.085	19.119
4	8	2	89.098	92.579	-3	9	-9	35.081	36.694
6	8	2	16.476	10.711	-1	9	-9	39.138	23.746
8	8	2	26.667	29.567	1	9	-9	128.268	126.049
-13	8	3	25.012	22.928	3	9	-9	73.215	71.988
-11	8	3	22.923	21.061	5	9	-9	22.976	22.670
-9	8	3	85.142	85.550	7	9	-9	45.955	48.084
-7	8	3	48.756	44.574	-12	9	-8	23.711	19.087
-5	8	3	27.732	24.867	-10	9	-8	63.488	62.237
-3	8	3	71.496	69.433	-8	9	-8	43.919	41.939
-1	8	3	36.293	39.783	-6	9	-8	27.467	25.002
1	8	3	52.752	54.868	-4	9	-8	19.122	17.969
3	8	3	63.484	64.610	-2	9	-8	39.915	39.936
5	8	3	12.333	13.055	0	9	-8	59.728	59.653
7	8	3	32.472	33.573	2	9	-8	29.061	26.359
-10	8	4	35.309	32.272	-13	9	-7	91.016	87.883
-8	8	4	61.813	68.143	-11	9	-7	154.569	148.328
-4	8	4	30.085	29.923	-9	9	-7	63.480	62.081
-2	8	4	118.850	122.414	-7	9	-7	39.037	38.596
0	8	4	52.285	52.717	-5	9	-7	25.772	28.397
2	8	4	16.549	15.647	-3	9	-7	11.695	8.561
4	8	4	56.370	56.500	-1	9	-7	95.378	95.831
-9	8	5	48.707	50.537	1	9	-7	26.114	23.471
-7	8	5	13.215	9.644	5	9	-7	22.321	20.875
-5	8	5	15.268	15.989	7	9	-7	29.764	28.186
-3	8	5	48.272	47.783	-12	9	-6	29.480	27.258
-1	8	5	19.142	25.613	-10	9	-6	20.683	15.675
1	8	5	25.829	28.297	-8	9	-6	83.053	82.122
-4	8	6	44.297	42.001	-6	9	-6	45.293	46.118
-2	8	6	39.947	41.012	-4	9	-6	170.618	167.585
0	8	6	44.272	46.288	-2	9	-6	101.569	100.405
-5	9	-13	27.122	25.560	2	9	-6	36.654	33.907
-3	9	-13	143.691	141.494	4	9	-6	93.073	90.145
-1	9	-13	90.801	88.191	6	9	-6	18.337	14.632
-8	9	-12	13.346	13.255	-13	9	-5	23.443	23.366
-4	9	-12	32.252	28.346	-11	9	-5	21.829	19.978
-2	9	-12	18.118	14.070	-9	9	-5	73.699	72.348
2	9	-12	38.423	35.310	-7	9	-5	21.232	20.913
-11	9	-11	34.667	36.333	-5	9	-5	71.244	71.479
-9	9	-11	21.028	16.001	-3	9	-5	49.512	48.070
-7	9	-11	43.020	43.409	1	9	-5	38.402	39.499
-5	9	-11	34.089	34.656	3	9	-5	72.033	72.303
1	9	-11	25.724	25.627	5	9	-5	82.073	82.974
5	9	-11	40.589	36.639	7	9	-5	34.984	34.912

Santalaraite Structure Factor Table (based on H-cell)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-14	9	-4	79.553	78.644	-5	9	1	88.516	86.621
-12	9	-4	22.183	19.814	-3	9	1	67.126	71.169
-8	9	-4	69.480	69.593	-1	9	1	63.577	67.861
-6	9	-4	88.073	85.317	1	9	1	11.915	13.313
-4	9	-4	47.041	45.161	3	9	1	38.260	39.161
-2	9	-4	36.740	36.047	5	9	1	42.012	44.953
0	9	-4	35.455	36.585	-10	9	2	28.878	29.574
4	9	-4	93.061	93.983	-8	9	2	20.699	17.442
6	9	-4	27.711	27.181	-6	9	2	26.898	27.746
8	9	-4	18.671	19.043	-2	9	2	43.732	45.028
-13	9	-3	21.390	16.733	2	9	2	43.821	45.249
-11	9	-3	40.776	39.763	-7	9	3	70.776	72.181
-9	9	-3	54.939	54.228	-5	9	3	13.589	14.638
-7	9	-3	63.411	66.736	-3	9	3	42.533	46.461
-5	9	-3	61.508	64.559	-1	9	3	13.402	6.179
-3	9	-3	37.667	38.330	1	9	3	36.179	33.122
-1	9	-3	38.057	39.189	-3	10	-11	51.195	49.525
1	9	-3	90.854	90.950	-6	10	-10	42.813	41.564
3	9	-3	60.780	61.469	-4	10	-10	95.337	94.501
5	9	-3	71.220	67.317	0	10	-10	41.350	38.892
7	9	-3	45.134	46.166	-9	10	-9	27.748	26.931
-14	9	-2	31.528	34.339	-7	10	-9	21.687	21.479
-12	9	-2	25.687	24.999	-5	10	-9	47.545	44.847
-8	9	-2	19.285	17.597	-1	10	-9	15.276	11.141
-6	9	-2	62.447	62.327	1	10	-9	31.707	32.313
-4	9	-2	12.146	9.963	-10	10	-8	58.825	55.909
-2	9	-2	34.419	33.018	-8	10	-8	18.923	18.330
0	9	-2	45.642	48.325	-4	10	-8	38.992	40.728
2	9	-2	69.252	74.059	-2	10	-8	40.329	39.242
4	9	-2	19.508	17.319	0	10	-8	12.459	14.209
6	9	-2	29.443	26.944	2	10	-8	36.138	33.148
-13	9	-1	71.943	71.414	-9	10	-7	101.305	100.264
-11	9	-1	94.594	93.804	-7	10	-7	73.415	73.748
-9	9	-1	54.671	54.395	-5	10	-7	27.366	30.547
-7	9	-1	21.341	18.801	-3	10	-7	41.927	42.449
-5	9	-1	11.752	16.537	-1	10	-7	78.195	79.568
-3	9	-1	24.280	22.220	1	10	-7	63.654	61.837
-1	9	-1	54.220	54.933	-10	10	-6	41.114	41.070
1	9	-1	49.150	48.501	-6	10	-6	14.866	13.094
3	9	-1	23.565	22.424	-4	10	-6	56.211	53.192
5	9	-1	19.585	14.893	-2	10	-6	14.110	8.995
7	9	-1	24.089	24.961	0	10	-6	105.484	105.414
-12	9	0	110.618	112.249	2	10	-6	22.211	21.187
-10	9	0	85.248	86.852	-11	10	-5	38.053	37.964
-8	9	0	19.276	21.020	-9	10	-5	39.541	40.312
-4	9	0	73.744	75.757	-7	10	-5	35.634	35.551
-2	9	0	88.268	90.255	-5	10	-5	38.354	35.106
0	9	0	68.276	66.105	-3	10	-5	12.374	10.886
4	9	0	17.557	22.759	-1	10	-5	55.744	56.405
6	9	0	69.358	69.318	1	10	-5	23.602	24.618
-11	9	1	49.081	50.589	3	10	-5	31.195	31.068
-9	9	1	22.191	23.427	-10	10	-4	13.508	9.904
-7	9	1	16.264	15.943	-8	10	-4	12.858	8.482



Santaclarita Structure Factor Table (based on B-cell)

H	K	L	F(OBS)	F(CALC)
-6	10	-4	69.069	66.727
-4	10	-4	40.870	37.507
0	10	-4	46.919	47.464
2	10	-4	40.809	38.612
-9	10	-3	46.402	47.802
-7	10	-3	102.480	102.023
-5	10	-3	120.358	120.764
-3	10	-3	49.301	49.956
-1	10	-3	24.476	21.344
3	10	-3	109.650	109.150
-8	10	-2	43.882	45.615
-6	10	-2	63.545	61.878
-4	10	-2	31.252	29.745
-2	10	-2	15.220	14.439
0	10	-2	39.894	38.947
2	10	-2	84.898	85.140
-7	10	-1	35.825	36.822
-5	10	-1	42.585	40.703
-3	10	-1	21.789	22.042
-1	10	-1	30.776	30.051
1	10	-1	35.297	35.377