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Crystal Structure of Joaquinite

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Abstract

The crystal structure of monoclinic joaquinite, ideal formula $NaFe^{2+}Ba_2RE_2Ti_2Si_8O_{26}OH \cdot H_2O$, has been determined by the Patterson method from 2630 diffractometer data, and refined by least-squares to a weighted R of 0.075. The space group is $C2$, and cell parameters are $a = 10.516 \pm 0.003$ Å, $b = 9.686 \pm 0.003$ Å, $c = 11.833 \pm 0.004$ Å, and $\beta = 109.67 \pm 0.003°$, with $Z = 2$. The new independent determination largely confirms a previous one by Cannillo, Mazzi, and Rossi (1972), but there are important differences, including the space group and several additional atoms found in the present study (Na, OH, H_2O). The principal structural unit is a four-membered Si_4O_{12} silicate ring, equivalents of which are linked by TiO_6 octahedra to form sheets parallel to (001). Sheets are stacked facing alternately up and down in the c direction; Ba atoms and water molecules occur midway between sheets on one level, and Na, Fe, and RE atoms on the alternate levels. The Ti octahedra are somewhat out of the plane of the sheets on the Ba–H_2O side, and they share an edge with each other to link sheets in the c direction. The Fe and Na polyhedra, which also link sheets, are very irregular; Fe is 5-coordinated, and Na is 6-coordinated. The orthorhombic form of joaquinite is evidently related to the monoclinic form by a type of unit-cell twinning on an (001) pseudo-mirror plane through Ba and H_2O. Macroscopic twinning of the monoclinic form on this plane and disordered stacking of monoclinic and orthorhombic forms also occur.

Introduction

Joaquinite occurs as small (~1 mm) honey-brown crystals associated with benitoite, neptunite, and natrolite in San Benito County, California (Louderback and Blasdale, 1909; Palache and Foshag, 1932), and also in Quebec (Bell, 1963) and South Greenland (Semenov *et al*, 1967). Satisfactory analyses have been obtained only recently, as the presence of rare-earth elements (RE) and strontium had not been recognized earlier. The composition of material from California and Greenland is somewhat different; Semenov *et al* (1967) suggested the formula $NaBa_2Fe^{2+}Ce_2Ti_2Si_8O_{26}OH$ for joaquinite from Greenland, and Laird and Albee (1972) suggested the formula $Ba_{8.1}(Sr_{1.7}RE_{6.5}Th_{0.1})_{8.3}$ $(Ca_{0.2}Na_{3.3}Fe_{3.1}Li_{0.8}Mg_{0.1})_{7.5}Ti_{8.1}Si_{32.0}O_{98.7}(OH)_{13.3}$ for material from California. However, the formulas are very similar in the ratios of the cations.

The existence of monoclinic as well as orthorhombic crystals of joaquinite has also been noted only recently (Laird and Albee, 1972; Cannillo, Mazzi, and Rossi, 1972). No chemical differences were detected between the two modifications, which occur intimately intergrown in the material from San Benito County. The 1 mm sized crystals show orthorhombic external morphology (Palache and Foshag, 1932), but X-ray studies by Laird and Albee (1972) and Cannillo *et al* (1972) have disclosed that these usually consist of finely twinned or disordered monoclinic joaquinite intermixed sometimes with orthorhombic joaquinite, the whole simulating orthorhombic symmetry.

A recent structural study of monoclinic joaquinite by Cannillo *et al* (1972) was unfortunately overlooked until the present study was entirely completed. Most of the important aspects of the structure proposed by them have been confirmed in the present study; however, it seems that they were unable to resolve all the atoms, largely due to the fact that they were forced to use intensity data from precession photographs of a twinned crystal. They also assumed that the space group was $C2/m$, instead of $C2$, as found in this study. A lower residual, more reasonable bond lengths, and better agreement with formulas proposed on the basis of microprobe data demonstrate that the present determination is a significant improvement over that of Cannillo, Mazzi,

Table 4.

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F (OBS)		F (CALC)	A (CALC,	B (CALC)
0	0	2	158.936		148.185	146.413	22.847
0	0	3	33.358		22.541	-22.540	-0.207
0	0	4	411.758		399.968	399.615	16.796
0	0	5	130.487		125.271	125.112	6.327
0	0	7	274.347		256.077	255.470	17.620
0	0	8	261.322		238.952	238.889	5.481
0	0	9	199.604		211.220	210.204	20.691
0	0	10	0.0	*	13.783	-13.642	-1.967
0	0	11	151.139		154.825	153.811	17.689
0	0	12	0.0	*	5.812	-5.277	-2.434
0	0	13	115.913		120.160	119.347	13.949
0	0	15	102.983		82.520	81.981	9.417
0	0	16	117.576		135.584	135.047	12.055
0	0	17	47.520		40.805	40.754	2.029
0	0	18	52.574		77.547	76.334	13.662
0	2	0	105.791		109.770	-108.091	-19.124
0	2	1	189.458		255.458	250.557	49.802
0	2	2	79.887		86.408	85.846	9.834
0	2	3	328.658		343.557	341.697	35.700
0	2	4	245.694		248.442	247.612	20.290
0	2	5	123.285		123.364	120.921	-24.430
0	2	6	187.322		203.008	202.924	-5.831
0	2	7	98.980		87.580	73.614	47.448
0	2	8	70.115		72.641	71.987	9.724
0	2	9	78.252		83.388	-67.022	49.614
0	2	10	272.143		275.483	275.283	-10.518
0	2	11	70.525		69.488	68.775	-9.934
0	2	12	175.277		165.369	165.198	-7.515
0	2	13	27.508		37.302	-5.809	36.847
0	2	14	144.555		136.829	135.676	17.725
0	2	15	19.120	*	36.596	35.134	-10.239
0	2	16	0.0	*	21.323	-20.958	-3.931
0	2	17	56.742		61.031	53.061	30.156
0	4	0	332.840		347.655	344.422	47.298
0	4	1	106.152		105.611	77.525	-71.719
0	4	2	236.804		251.667	248.212	41.562
0	4	3	78.066		71.346	68.328	20.532
0	4	4	70.441		86.698	71.777	48.627
0	4	5	69.202		62.652	62.583	2.940
0	4	6	54.465		66.951	62.666	23.567
0	4	7	251.666		253.206	252.523	-18.588
0	4	8	82.051		89.603	88.900	-11.205
0	4	9	233.061		236.140	236.078	5.408
0	4	10	80.057		72.511	-67.463	26.581
0	4	11	138.043		140.055	139.768	8.974
0	4	12	46.706		49.970	-49.961	-0.933
0	4	13	157.670		152.866	147.518	40.083
0	4	14	18.243	*	19.383	18.591	5.482
0	4	15	72.269		73.026	69.965	-20.923
0	4	16	85.508		89.112	89.025	-3.953
0	4	17	64.099		60.445	55.481	23.990
0	6	0	198.547		196.382	-151.953	124.403

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
0	6	2	158.952		153.564	142.614	56.950
0	6	3	233.698		254.998	250.416	-48.123
0	6	4	70.743		61.202	61.093	-3.657
0	6	5	127.791		147.966	147.667	-9.395
0	6	6	210.127		200.238	192.797	54.081
0	6	7	43.578		44.715	30.451	32.744
0	6	8	70.091		67.249	67.208	2.356
0	6	9	22.687		10.856	-9.460	5.326
0	6	10	217.254		218.078	210.114	58.394
0	6	11	40.821		41.543	31.597	-26.972
0	6	12	135.161		141.133	140.945	-7.274
0	6	13	31.828		29.912	27.254	-12.328
0	6	14	100.776		104.347	95.728	41.525
0	6	15	28.795		24.538	22.260	-10.324
0	6	16	25.266		38.766	C.922	38.755
0	8	0	298.984		304.196	303.297	-23.366
0	8	1	77.706		64.882	62.569	-17.172
0	8	2	135.901		156.392	156.079	-9.892
0	8	3	36.006		39.229	-14.493	36.453
0	8	4	123.482		141.757	138.141	31.814
0	8	5	136.500		116.327	116.273	-5.546
0	8	6	57.160		73.522	72.444	12.544
0	8	7	98.484		97.262	97.251	1.460
0	8	8	97.229		113.169	105.894	-39.921
0	8	9	173.845		177.385	176.251	-20.033
0	8	10	23.553		24.074	7.477	22.884
0	8	11	65.561		69.216	60.608	33.429
0	8	12	30.026		26.626	26.542	-2.112
0	8	13	94.152		96.791	95.419	16.241
0	8	14	13.971	*	21.561	21.158	-4.148
0	8	15	60.555		55.166	54.724	-6.969
0	10	0	60.958		53.502	-26.259	46.615
0	10	1	150.670		152.132	149.874	26.113
0	10	2	74.937		68.309	60.721	-31.291
0	10	3	126.481		137.421	134.513	28.124
0	10	4	79.919		70.079	68.058	-16.706
0	10	5	106.250		128.410	127.067	-18.519
0	10	6	122.634		110.812	108.169	-24.059
0	10	7	62.774		67.201	12.602	66.009
0	10	8	87.959		81.015	79.256	16.793
0	10	9	30.209		30.758	24.093	19.120
0	10	10	108.896		113.865	112.243	-19.152
0	10	11	37.416		34.790	32.480	12.466
0	10	12	113.685		114.593	109.545	-33.638
0	10	13	32.645		28.053	27.897	2.950
0	12	0	85.270		85.466	84.590	12.209
0	12	1	62.770		61.798	61.748	-2.478
0	12	2	88.648		99.640	99.020	-11.099
0	12	3	63.801		51.530	36.541	36.333
0	12	4	79.391		82.504	46.251	68.320
0	12	5	83.154		64.232	64.124	-3.721
0	12	6	23.576		41.038	40.947	-2.732
0	12	7	95.968		83.043	82.452	9.885

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
0	12	8	39.997		49.178	48.342	9.032
0	12	9	113.538		111.737	109.355	-22.948
0	12	10	29.831		19.499	-10.601	16.366
0	12	11	69.947		70.187	65.073	26.298
0	14	0	31.173		66.750	4.233	66.615
0	14	1	72.405		69.301	69.176	4.160
0	14	2	62.671		52.836	52.825	1.072
0	14	3	67.709		76.190	75.453	-10.569
0	14	4	50.018		49.793	49.668	3.532
0	14	5	45.299		53.938	53.829	-3.423
0	14	6	73.276		58.323	58.193	3.890
0	14	7	20.128	*	32.514	28.589	15.486
0	14	8	73.060		72.707	61.292	39.111
1	15	0	23.070		14.438	-11.671	8.499
1	15	1	6.751	*	22.551	20.888	8.502
1	15	2	38.038		28.165	9.563	26.492
1	15	3	27.714		22.770	-5.172	-22.175
1	15	4	23.848		31.168	-31.132	-1.505
1	13	0	75.342		51.888	-12.316	-50.405
1	13	1	63.466		53.421	37.920	37.627
1	13	2	50.755		41.640	2.371	-41.541
1	13	3	54.745		48.277	-25.019	41.288
1	13	4	38.815		37.263	21.352	-30.539
1	13	5	72.720		79.136	44.175	65.659
1	13	6	26.643		36.157	-23.779	-27.239
1	13	7	72.191		71.705	-70.514	-13.016
1	13	8	19.744		25.285	-7.598	-24.116
1	13	9	7.645	*	8.512	2.740	8.059
1	11	0	62.459		38.813	13.487	36.394
1	11	1	49.650		32.400	-24.641	-21.037
1	11	2	79.576		69.367	17.485	67.127
1	11	3	104.046		98.959	-35.665	-92.309
1	11	4	34.185		29.869	-20.409	21.809
1	11	5	44.559		55.937	-31.057	-46.523
1	11	6	36.987		41.071	3.329	40.936
1	11	7	28.294		35.871	18.243	-30.886
1	11	8	18.113		11.663	1.255	11.596
1	11	9	53.246		49.137	-40.555	27.744
1	11	10	35.447		26.729	-26.575	-2.863
1	11	11	25.953		31.478	-19.519	-24.695
1	11	12	59.314		56.460	-23.265	-51.444
1	9	0	48.536		22.904	1.640	-22.845
1	9	1	47.045		45.128	42.186	-16.027
1	9	2	78.281		66.634	-36.318	-55.866
1	9	3	84.804		86.807	31.822	80.764
1	9	4	33.511		35.456	15.199	-32.033
1	9	5	44.215		53.594	12.016	52.230
1	9	6	64.206		66.788	-60.376	-28.554
1	9	7	53.320		48.861	-44.498	-20.180
1	9	8	29.838		41.354	1.762	-41.316
1	9	9	42.487		32.940	-13.881	-29.872
1	9	10	57.397		43.846	-28.532	33.292
1	9	11	37.332		37.373	-12.620	-35.178

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
1	9	12	61.629	59.214	-0.938	59.206
1	9	13	45.011	40.091	-12.174	-38.198
1	9	14	46.621	53.305	-37.776	37.609
1	7	0	122.608	96.277	-2.173	96.252
1	7	1	80.191	56.620	-20.876	-52.631
1	7	2	117.681	110.182	-33.135	105.082
1	7	3	87.781	87.855	45.244	-75.309
1	7	4	52.165	54.818	-28.298	46.949
1	7	5	143.962	157.566	-57.198	-146.818
1	7	6	77.152	88.451	-13.684	87.386
1	7	7	101.099	103.815	86.626	57.215
1	7	8	24.051	30.468	-27.711	12.667
1	7	9	56.077	54.303	-53.433	9.684
1	7	10	57.656	52.090	-47.324	-21.769
1	7	11	43.542	36.090	18.171	31.181
1	7	12	103.719	112.197	-47.398	-101.694
1	7	13	73.142	70.412	-37.602	59.531
1	7	14	55.086	50.616	-16.744	-47.766
1	7	15	83.133	75.845	16.717	73.980
1	5	0	116.212	116.194	95.569	-66.088
1	5	1	57.227	36.179	4.421	35.908
1	5	2	158.876	152.732	18.434	-151.615
1	5	3	264.798	268.328	12.370	268.042
1	5	4	60.536	64.523	30.884	-56.651
1	5	5	56.271	66.290	-6.750	65.946
1	5	6	73.207	80.019	5.772	-79.810
1	5	7	76.839	90.648	-73.747	52.712
1	5	8	66.232	70.303	-20.730	-67.177
1	5	9	40.481	41.737	-19.908	-36.683
1	5	10	41.438	45.528	25.537	37.692
1	5	11	27.357	31.905	-30.139	10.467
1	5	12	72.337	68.383	-31.789	60.545
1	5	13	50.550	51.832	-29.550	-42.583
1	5	14	58.817	51.186	-12.445	49.650
1	5	15	108.269	103.746	-45.921	-93.030
1	5	16	37.329	38.455	-35.076	15.764
1	3	0	252.811	233.361	43.718	229.229
1	3	1	217.254	211.188	-91.011	-190.571
1	3	2	140.218	131.043	52.613	120.016
1	3	3	294.886	291.583	-90.566	-277.167
1	3	4	103.554	108.145	-2.926	108.105
1	3	5	189.114	197.350	-49.012	-191.167
1	3	6	132.502	131.111	26.521	128.401
1	3	7	23.277	30.716	-6.598	-29.999
1	3	8	70.430	70.697	-66.143	24.964
1	3	9	39.570	43.835	-43.777	2.252
1	3	10	8.032 *	18.112	9.115	-15.651
1	3	11	61.457	60.692	-60.566	-3.910
1	3	12	134.728	137.799	-35.375	-133.181
1	3	13	63.775	68.922	-42.895	53.955
1	3	14	35.224	41.462	-7.676	-40.746
1	3	15	88.592	86.802	-39.487	77.301

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
1	3	17	55.968		55.094	-46.716	29.205
1	1	1	17.879		18.890	6.907	17.582
1	1	2	133.972		143.867	22.047	-142.168
1	1	3	198.898		198.692	25.430	197.058
1	1	4	33.024		33.201	-13.917	-30.144
1	1	5	156.387		147.679	-43.558	141.109
1	1	6	141.429		127.713	2.707	-127.685
1	1	7	41.192		47.451	-41.893	-22.283
1	1	8	79.055		73.467	-27.369	-68.178
1	1	9	35.161		41.162	14.228	-38.625
1	1	10	87.897		95.583	-53.074	79.494
1	1	11	61.377		63.668	-39.466	-49.961
1	1	12	111.642		121.116	-47.637	111.355
1	1	13	90.252		98.077	31.426	-92.906
1	1	14	92.517		94.623	-66.997	66.820
1	1	15	120.801		126.149	-46.830	-117.135
1	1	16	42.949		44.522	-25.736	36.329
1	1	17	57.819		50.764	6.174	-50.387
2	0	0	164.689		155.854	-155.229	-13.933
2	0	1	231.913		219.010	-218.767	-10.312
2	0	2	80.683		67.418	-66.787	-9.197
2	0	3	259.102		245.593	-244.737	-20.497
2	0	4	63.074		51.374	-51.249	-3.585
2	0	5	372.787		362.723	-361.935	-23.887
2	0	6	191.968		187.893	187.803	5.819
2	0	7	282.406		272.817	-271.840	-23.068
2	0	9	176.402		175.327	-174.029	-21.288
2	0	10	28.260		38.157	38.127	-1.509
2	0	11	187.585		176.165	-175.264	-17.796
2	0	12	114.764		131.811	-131.464	-9.562
2	0	13	62.327		50.670	-50.290	-6.198
2	0	14	16.280	*	28.378	-26.237	-10.813
2	0	15	33.522		11.212	-11.130	1.358
2	0	16	104.122		119.123	-118.116	-15.457
2	0	17	17.545	*	21.521	21.326	2.891
2	2	0	91.430		84.983	-82.281	-21.262
2	2	1	380.923		416.052	-415.375	23.715
2	2	2	151.569		148.734	-146.749	-24.215
2	2	3	25.659		22.716	-21.885	-6.086
2	2	4	190.774		194.308	-190.605	-37.754
2	2	5	111.263		122.141	-117.232	34.282
2	2	6	277.124		280.219	-280.126	-7.246
2	2	7	34.907		17.506	12.588	-12.166
2	2	8	246.024		239.593	-238.262	-25.215
2	2	9	78.896		77.557	-75.302	18.565
2	2	10	148.834		134.813	-131.586	-29.317
2	2	11	17.132	*	35.528	-34.775	-7.278
2	2	12	66.720		56.137	-53.514	-16.957
2	2	13	86.227		98.098	-94.293	27.057
2	2	14	89.489		75.668	-66.719	-35.697
2	2	15	104.356		129.443	-129.306	-5.959
2	2	16	14.960	*	10.930	10.836	-1.432

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
2	4	1	28.933		20.389	-11.025	-17.151
2	4	2	169.088		197.288	-193.808	36.890
2	4	3	251.713		250.811	-249.132	-28.970
2	4	4	167.500		181.511	-180.471	-19.402
2	4	5	183.616		186.873	-184.693	-28.461
2	4	6	42.773		42.818	29.816	30.731
2	4	7	244.391		258.201	-250.794	-61.401
2	4	8	38.957		39.537	-39.284	-4.468
2	4	9	110.053		118.057	-117.914	5.802
2	4	10	64.271		57.811	-57.437	6.567
2	4	11	157.662		162.680	-159.314	-32.922
2	4	12	136.718		132.153	-131.938	7.528
2	4	13	21.610		11.752	-11.588	-1.951
2	4	14	93.557		98.957	-96.924	-19.957
2	4	15	26.864		17.592	-4.570	-16.988
2	4	16	109.244		114.766	-114.618	5.822
2	6	0	126.867		109.905	-108.193	19.322
2	6	1	169.370		190.215	-183.119	-51.469
2	6	2	149.266		130.857	-128.141	26.526
2	6	3	85.015		89.161	-54.164	-70.823
2	6	4	148.517		146.929	-141.264	40.406
2	6	5	31.007		33.509	-24.939	-22.382
2	6	6	242.009		244.529	-241.996	35.100
2	6	7	49.046		52.286	-31.527	-41.711
2	6	8	158.792		169.684	-169.246	12.176
2	6	9	37.404		40.542	-39.586	8.751
2	6	10	133.654		146.794	-146.159	-13.642
2	6	11	55.382		56.679	-28.425	-49.036
2	6	12	26.059		23.498	-18.640	14.308
2	6	13	88.730		83.673	-82.843	11.761
2	6	14	71.130		72.741	-71.282	-14.495
2	6	15	114.032		114.578	-113.646	-14.581
2	8	0	124.755		135.507	-126.352	-48.963
2	8	1	71.464		56.294	-43.983	-35.136
2	8	2	45.454		72.395	-69.857	18.999
2	8	3	231.542		219.215	-217.163	29.922
2	8	4	67.938		76.318	-60.182	-46.932
2	8	5	143.944		145.853	-143.521	-25.977
2	8	6	6.833	*	6.631	0.729	-6.591
2	8	7	155.651		161.641	-159.603	-25.586
2	8	8	32.979		36.578	6.267	-36.037
2	8	9	95.704		107.023	-106.887	-5.389
2	8	10	35.816		34.730	-31.331	14.985
2	8	11	117.857		124.308	-123.195	-16.602
2	8	12	68.912		67.276	-67.055	-5.438
2	8	13	52.880		59.780	-59.187	-8.397
2	8	14	46.268		46.448	-42.510	-18.718
2	10	0	88.015		72.885	-72.876	-1.136
2	10	1	81.130		102.552	-102.092	-9.700
2	10	2	136.275		117.056	-103.929	-53.860
2	10	3	17.695		32.147	-31.403	6.879
2	10	4	96.534		88.566	-78.793	-40.442
2	10	5	18.096		19.175	-14.910	-12.057

JCAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
2	10	6	175.248		165.439	-164.776	14.796
2	10	7	17.489	*	32.809	-31.117	10.395
2	10	8	100.178		110.804	-108.891	-20.501
2	10	9	46.487		38.865	-38.703	3.549
2	10	10	96.889		102.510	-98.073	-29.832
2	10	11	25.787		13.232	-8.673	-9.993
2	10	12	37.273		47.391	-27.621	-38.510
2	12	0	84.365		85.555	-85.021	-9.540
2	12	1	38.606		43.352	-15.419	-40.518
2	12	2	73.223		97.947	-93.431	29.399
2	12	3	128.040		113.232	-106.781	37.675
2	12	4	55.304		71.437	-71.311	-4.244
2	12	5	85.937		83.098	-79.385	-24.561
2	12	6	41.731		46.372	-46.039	-5.551
2	12	7	78.862		75.243	-74.903	7.136
2	12	8	40.443		38.529	-15.456	-35.293
2	12	9	64.068		72.981	-69.250	-23.038
2	12	10	63.943		64.459	-51.313	39.012
2	14	0	68.990		58.472	-47.231	34.470
2	14	1	52.887		72.276	-70.605	-15.453
2	14	2	72.191		59.936	-54.409	-25.141
2	14	3	51.616		50.813	-41.352	-29.530
2	14	4	54.562		43.320	-43.284	1.768
2	14	5	33.174		38.003	-29.039	-24.514
2	14	6	91.813		84.161	-82.109	18.472
2	14	7	27.840		29.187	-28.987	3.409
3	15	0	32.893		23.159	19.097	-13.101
3	15	1	19.428	*	11.745	6.297	9.914
3	15	2	60.402		66.517	-54.927	-37.517
3	13	0	40.728		33.746	-30.035	15.385
3	13	1	0.0	*	3.274	-1.353	2.982
3	13	2	11.795	*	28.160	21.701	17.946
3	13	3	19.235		16.101	-2.420	-15.918
3	13	4	8.592	*	14.459	9.287	11.082
3	13	5	32.219		23.591	-15.584	17.710
3	13	6	45.919		39.236	-16.265	-35.706
3	13	7	14.664	*	1.710	-1.707	0.102
3	13	8	37.163		27.707	-14.681	-23.498
3	11	0	51.001		51.061	35.333	-36.862
3	11	1	36.587		50.513	-26.971	42.710
3	11	2	63.221		72.535	-55.686	-46.480
3	11	3	63.582		51.589	-46.676	-21.974
3	11	4	33.508		30.452	25.349	-16.875
3	11	5	24.384		31.389	-25.242	18.658
3	11	6	22.361		12.009	-4.789	11.012
3	11	7	38.119		24.574	5.810	-23.878
3	11	8	69.015		72.300	40.896	59.622
3	11	9	48.087		45.801	-18.352	-41.964
3	11	10	26.409		17.922	-15.735	8.580
3	11	11	54.943		57.508	-12.558	-56.120
3	9	0	62.193		66.985	-57.331	34.449
3	9	1	51.182		51.189	-22.707	-45.878
3	9	2	89.926		94.180	5.107	94.025

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
3	9	3	56.930		63.642	11.553	-62.585
3	9	4	35.982		42.340	-30.512	29.355
3	9	5	15.645		18.195	-2.127	-18.070
3	9	6	17.504	*	2.958	2.581	1.447
3	9	7	28.661		34.367	5.511	-33.922
3	9	8	79.445		79.145	-61.464	-49.861
3	9	9	74.109		72.929	14.684	71.435
3	9	10	57.070		54.308	42.572	-33.719
3	9	11	50.260		50.113	34.458	36.386
3	9	12	26.287		26.709	-21.144	-16.318
3	9	13	23.274		22.106	0.648	22.097
3	7	0	95.354		103.486	-0.241	-103.485
3	7	1	47.667		55.341	-55.336	-0.732
3	7	2	72.983		81.439	-47.034	-66.484
3	7	3	96.870		112.881	17.715	111.482
3	7	4	60.118		85.695	-31.991	-79.500
3	7	5	15.753		4.019	0.781	3.943
3	7	6	60.756		51.060	-19.103	47.352
3	7	7	31.057		35.542	33.913	10.636
3	7	8	71.208		62.560	10.928	61.598
3	7	9	77.517		75.353	4.514	-75.218
3	7	10	64.971		59.592	2.903	59.521
3	7	11	59.171		63.870	8.605	-63.288
3	7	12	50.912		49.532	-11.523	48.173
3	7	13	45.926		47.494	41.523	-23.055
3	7	14	13.149	*	20.981	3.151	20.743
3	5	0	81.210		93.061	-71.352	59.742
3	5	1	110.381		112.570	-48.195	-101.731
3	5	2	104.536		122.249	39.851	115.571
3	5	3	28.895		16.743	16.526	-2.690
3	5	4	29.916		23.677	-23.642	-1.284
3	5	5	52.468		55.690	-52.587	18.332
3	5	6	49.202		59.603	59.254	-6.441
3	5	7	15.086	*	9.864	0.969	9.816
3	5	8	113.962		116.116	-20.009	-114.379
3	5	9	123.267		126.250	0.968	126.247
3	5	10	45.528		53.296	34.602	-40.536
3	5	11	63.372		72.440	12.374	71.375
3	5	12	63.071		69.208	28.099	-63.247
3	5	13	77.591		75.435	-2.068	75.407
3	5	14	55.797		56.301	39.797	-39.824
3	5	15	0.0	*	9.537	-7.136	-6.328
3	3	0	171.845		172.846	-36.999	-168.840
3	3	1	104.961		108.921	-73.814	80.096
3	3	2	93.520		101.320	9.795	-100.845
3	3	3	84.029		84.337	-73.290	41.728
3	3	4	89.017		98.626	-1.326	-98.617
3	3	5	64.799		55.460	-36.223	-41.997
3	3	6	95.453		86.404	2.031	86.381
3	3	7	73.763		69.001	-32.591	-60.819
3	3	8	99.765		100.362	41.423	91.415
3	3	9	117.145		119.012	3.702	-118.954
3	3	10	85.807		86.420	-9.444	85.903

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
3	3	11	127.728		121.071	-13.497	-120.316
3	3	12	79.760		79.730	39.217	69.418
3	3	13	66.634		63.195	22.109	-59.202
3	3	14	47.311		47.529	-9.395	46.591
3	3	15	23.377		13.014	12.897	-1.747
3	3	16	41.458		47.437	43.881	18.021
3	1	0	167.400		172.101	-94.086	144.106
3	1	1	84.871		83.695	32.653	-77.063
3	1	2	194.197		189.000	-66.660	176.855
3	1	3	199.813		195.647	-29.471	-193.414
3	1	4	102.034		94.707	-49.023	81.032
3	1	5	69.895		65.590	64.800	10.154
3	1	6	13.503	*	11.441	-4.377	-10.571
3	1	7	66.505		57.456	-52.239	-23.922
3	1	8	108.475		107.287	14.087	-106.358
3	1	9	126.876		130.682	37.540	125.174
3	1	10	58.675		63.932	5.170	-63.722
3	1	11	68.396		64.664	-13.195	63.304
3	1	12	70.723		69.559	37.377	-58.664
3	1	13	75.501		71.202	20.490	68.191
3	1	14	43.141		32.206	-3.933	-31.965
3	1	15	38.698		49.544	35.175	-34.890
3	1	16	34.648		23.685	23.647	-1.345
4	0	0	39.553		34.505	34.000	5.882
4	0	1	309.841		279.780	279.298	16.414
4	0	2	132.434		129.632	129.632	-0.220
4	0	3	237.993		223.134	222.273	19.585
4	0	4	43.606		38.070	-38.039	-1.526
4	0	5	250.291		227.065	226.092	21.005
4	0	6	224.062		220.466	220.382	6.073
4	0	7	208.705		188.523	187.803	16.458
4	0	8	65.029		74.552	73.957	9.401
4	0	9	80.391		65.828	65.590	5.601
4	0	10	135.648		145.901	145.251	13.760
4	0	11	0.0	*	5.074	-4.779	-1.706
4	0	12	163.641		170.706	169.538	19.931
4	0	13	0.0	*	10.121	-9.730	-2.787
4	0	14	183.233		186.227	184.813	22.908
4	0	15	14.490	*	14.799	14.691	-1.788
4	2	0	242.655		242.589	232.796	68.231
4	2	1	50.861		56.118	54.667	12.678
4	2	2	339.252		351.124	349.948	-28.709
4	2	3	18.449		16.164	9.560	-13.034
4	2	4	220.177		229.516	227.679	28.985
4	2	5	95.364		101.332	63.965	78.591
4	2	6	163.687		171.779	166.244	-43.252
4	2	7	44.564		37.342	-36.853	.023
4	2	8	148.820		137.622	134.675	.30
4	2	9	158.726		163.312	156.132	.93
4	2	10	92.783		82.365	81.957	-8.187
4	2	11	126.571		122.682	122.613	-4.123
4	2	12	23.455		20.573	20.353	-2.998
4	2	13	157.819		157.196	154.432	29.353

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
4	2	14	40.927	38.333	-37.688	-7.004
4	2	15	94.958	87.018	79.211	36.024
4	4	0	32.227	14.381	-9.001	11.216
4	4	1	166.199	160.175	159.489	14.813
4	4	2	50.411	40.675	-38.260	-13.807
4	4	3	247.285	253.881	253.551	12.944
4	4	4	59.688	60.307	-19.750	56.981
4	4	5	211.943	227.397	226.221	23.100
4	4	6	33.791	35.675	22.971	-27.295
4	4	7	200.742	211.834	210.733	-21.572
4	4	8	75.550	73.390	63.404	36.960
4	4	9	64.063	67.140	64.462	18.774
4	4	10	63.193	66.970	64.831	-16.793
4	4	11	27.035	30.000	21.998	20.398
4	4	12	142.871	141.929	133.392	48.484
4	4	13	22.845	15.741	-5.657	-14.689
4	4	14	126.664	125.907	125.653	-7.990
4	4	15	54.537	51.127	50.484	8.081
4	6	0	210.296	194.258	194.241	-2.567
4	6	1	95.714	105.925	93.753	49.300
4	6	2	209.264	204.090	192.520	67.742
4	6	3	44.525	64.747	26.876	-58.905
4	6	4	228.025	233.178	231.847	-24.876
4	6	5	35.423	31.358	24.925	19.029
4	6	6	110.178	116.867	96.550	65.848
4	6	7	17.829	10.454	9.727	-3.830
4	6	8	130.010	143.038	135.214	46.658
4	6	9	117.379	118.902	117.780	-16.299
4	6	10	34.502	47.969	47.268	8.167
4	6	11	125.838	127.294	126.708	-12.199
4	6	12	38.795	42.010	25.641	33.277
4	6	13	104.904	106.317	105.830	-10.166
4	6	14	31.204	32.469	-28.198	16.097
4	8	0	56.989	82.488	78.003	-26.828
4	8	1	154.790	138.974	138.794	-7.076
4	8	2	29.455	27.717	20.221	18.956
4	8	3	132.471	130.332	125.416	35.459
4	8	4	47.461	47.680	46.925	8.455
4	8	5	123.121	139.711	139.461	8.363
4	8	6	91.297	88.656	83.146	-30.769
4	8	7	124.453	136.916	136.731	-7.124
4	8	8	82.190	77.138	76.336	11.095
4	8	9	21.439	22.105	18.698	11.790
4	8	10	85.171	82.191	80.424	-16.949
4	8	11	38.283	45.798	31.636	33.115
4	8	12	115.292	118.118	112.760	35.170
4	8	13	0.0 *	9.049	2.749	-8.622
4	10	0	160.403	149.285	146.256	-29.921
4	10	1	75.976	85.010	82.049	22.240
4	10	2	123.734	121.824	121.820	-0.895
4	10	3	32.783	35.913	33.432	-13.118
4	10	4	140.001	146.832	140.337	-43.188
4	10	5	53.551	53.296	16.714	50.607

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
4	10	6	75.366		83.000	79.012	25.420
4	10	7	44.714		42.056	40.737	10.449
4	10	8	63.607		78.279	77.337	-12.112
4	10	9	95.582		88.418	82.317	32.274
4	10	10	54.032		54.902	54.812	3.130
4	10	11	95.812		98.210	93.131	-31.174
4	12	0	36.199		39.821	37.934	12.112
4	12	1	81.895		64.396	61.534	-18.983
4	12	2	36.528		35.398	-5.823	34.916
4	12	3	125.935		113.711	106.412	40.083
4	12	4	44.063		39.988	31.237	24.805
4	12	5	84.678		94.744	94.743	-0.326
4	12	6	31.904		26.814	26.389	-4.754
4	12	7	97.810		99.658	98.395	-15.817
4	12	8	23.517		27.984	26.497	9.002
4	12	9	31.011		43.416	34.237	26.699
4	14	0	89.676		74.625	74.419	-5.540
4	14	1	18.315	*	27.827	27.475	4.411
4	14	2	88.118		83.105	80.751	19.639
4	14	3	35.650		45.554	39.997	-21.803
4	14	4	85.654		74.375	72.863	-14.920
4	14	5	18.021	*	2.383	-0.252	2.370
5	13	0	49.598		37.776	37.699	-2.414
5	13	1	14.065	*	35.706	12.509	33.443
5	13	2	39.997		35.968	35.880	2.511
5	13	3	39.563		41.754	41.159	7.026
5	13	4	33.778		34.442	23.148	25.503
5	13	5	41.879		39.429	-27.542	-28.215
5	13	6	0.0	*	4.937	4.732	-1.410
5	11	0	71.473		86.616	48.049	72.067
5	11	1	24.537		14.999	10.530	-10.680
5	11	2	69.107		48.952	-0.674	-48.947
5	11	3	13.635	*	8.241	-5.497	-6.140
5	11	4	0.0	*	17.034	11.318	12.731
5	11	5	63.104		59.228	18.373	56.306
5	11	6	68.870		65.954	53.967	-37.914
5	11	7	37.398		35.151	-0.338	35.149
5	11	8	13.195	*	7.342	1.443	-7.199
5	11	9	13.663	*	13.394	-13.272	1.806
5	9	0	28.441		40.445	6.111	-39.981
5	9	1	24.547		43.902	25.866	35.473
5	9	2	95.252		78.814	51.220	59.902
5	9	3	67.216		65.643	61.778	-22.192
5	9	4	56.318		45.251	23.581	38.621
5	9	5	91.931		84.032	-10.528	-83.370
5	9	6	47.803		40.525	-9.745	39.336
5	9	7	56.556		58.871	4.524	-58.697
5	9	8	52.889		62.153	-2.377	62.108
5	9	9	53.866		56.755	32.582	-46.471
5	9	10	49.491		51.895	15.256	49.592
5	9	11	17.745	*	8.958	8.586	2.557
5	7	0	26.397		37.153	17.117	32.975
5	7	1	41.517		40.759	36.553	-18.032

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
5	7	2	54.024		40.404	29.306	-27.814
5	7	3	39.837		20.842	17.330	11.579
5	7	4	50.781		44.510	-17.538	-40.910
5	7	5	161.377		165.047	72.981	148.034
5	7	6	70.767		73.434	45.336	-57.769
5	7	7	65.978		68.641	15.834	66.790
5	7	8	37.373		45.333	-11.793	-43.772
5	7	9	65.082		74.650	27.176	69.528
5	7	10	75.273		83.933	-2.747	-83.888
5	7	11	29.951		26.671	-26.650	-1.064
5	7	12	28.249		16.650	-10.313	13.072
5	7	13	46.674		41.755	31.330	27.603
5	5	0	138.867		154.773	25.740	-152.618
5	5	1	72.322		101.253	60.630	81.093
5	5	2	197.039		189.286	106.310	156.612
5	5	3	35.482		40.230	39.939	-4.826
5	5	4	41.913		35.543	35.532	0.903
5	5	5	77.894		72.655	-2.193	-72.622
5	5	6	60.324		67.857	33.009	59.287
5	5	7	77.270		81.860	8.353	-81.433
5	5	8	44.181		46.871	10.879	45.591
5	5	9	21.831		12.816	8.751	-9.363
5	5	10	83.984		87.235	19.880	84.940
5	5	11	0.0	*	18.745	18.493	3.059
5	5	12	8.630	*	20.724	12.706	-16.371
5	5	13	28.359		25.201	-21.857	-12.544
5	5	14	50.932		55.140	-22.725	-50.239
5	3	0	144.823		164.782	85.397	140.927
5	3	1	66.100		67.022	41.594	-52.553
5	3	2	137.160		137.415	44.066	-130.158
5	3	3	54.225		62.398	-15.543	-60.431
5	3	4	36.225		35.748	22.138	-28.068
5	3	5	161.848		164.433	40.078	159.474
5	3	6	78.330		81.264	45.162	-67.559
5	3	7	56.009		61.747	-10.878	60.781
5	3	8	65.788		68.326	45.027	-51.391
5	3	9	65.185		57.814	-29.689	49.608
5	3	10	124.275		118.624	-0.517	-118.623
5	3	11	19.701	*	22.068	-4.218	-21.661
5	3	12	50.440		43.011	13.983	40.675
5	3	13	11.944	*	22.531	-20.721	8.848
5	3	14	38.801		45.978	3.795	45.821
5	1	0	115.918		112.835	79.412	-80.159
5	1	1	91.722		100.264	78.217	62.730
5	1	2	163.138		156.005	13.538	155.417
5	1	3	34.584		40.533	35.605	-19.370
5	1	4	87.464		83.313	74.447	37.399
5	1	5	173.510		172.709	66.312	-159.471
5	1	6	118.453		114.356	-65.130	93.996
5	1	7	154.312		138.431	43.344	-131.470
5	1	8	106.586		93.869	28.403	89.468
5	1	9	95.589		86.653	31.015	-80.912
5	1	10	151.310		129.184	-41.401	122.370

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F (OBS)		F (CALC)	A (CALC)	B (CALC)
5	1	11	31.239		26.676	26.388	3.906
5	1	12	14.799	*	17.414	9.706	-14.458
5	1	13	57.441		43.347	-21.601	-37.581
5	1	14	45.432		61.473	-7.588	-61.003
5	1	15	41.731		47.664	13.313	45.767
6	0	0	26.805		29.566	29.279	4.104
6	0	1	314.206		292.854	-291.827	-24.499
6	0	2	23.189		15.355	15.354	0.197
6	0	3	342.316		302.596	-301.916	-20.274
6	0	4	14.556	*	3.650	2.593	-2.569
6	0	5	38.237		22.955	-20.945	-9.392
6	0	6	64.517		69.790	-69.197	-9.082
6	0	7	69.018		59.165	-59.024	-4.085
6	0	8	140.403		140.756	-139.719	-17.054
6	0	9	43.813		41.668	-41.627	-1.845
6	0	10	179.956		178.783	-177.504	-21.349
6	0	11	20.210	*	21.887	-21.882	0.433
6	0	12	86.091		86.052	-84.627	-15.596
6	0	13	20.823	*	14.409	14.404	0.371
6	0	14	76.436		63.517	-62.757	-9.793
6	2	0	243.681		240.041	-238.792	-24.461
6	2	1	91.354		87.733	84.237	-24.517
6	2	2	129.242		128.810	-126.300	-25.302
6	2	3	52.708		64.828	-60.120	24.254
6	2	4	170.939		174.540	-174.504	-3.535
6	2	5	118.926		129.09[illegible]	-128.372	-13.671
6	2	6	111.679		109.0[illegible]	-105.757	-26.705
6	2	7	177.661		188.128	-185.726	29.968
6	2	8	17.566	*	15.445	0.593	-15.434
6	2	9	113.157		116.618	-113.480	-26.874
6	2	10	28.359		35.187	26.364	-23.304
6	2	11	137.598		132.695	-130.997	21.158
6	2	12	34.028		29.819	-27.455	-11.636
6	2	13	151.620		147.195	-145.813	-20.118
6	2	14	33.177		41.366	-41.366	0.059
6	4	0	41.192		48.723	-22.806	43.056
6	4	1	251.227		262.941	-261.622	26.307
6	4	2	122.293		112.539	-112.391	-5.771
6	4	3	176.181		193.613	-187.666	-47.617
6	4	4	50.789		44.085	-31.901	30.427
6	4	5	63.364		68.010	-61.697	-28.615
6	4	6	140.489		143.207	-138.138	-37.764
6	4	7	14.987	*	4.570	2.959	-3.483
6	4	8	154.346		157.801	-157.335	12.111
6	4	9	43.182		43.466	-43.403	-2.330
6	4	10	206.305		213.394	-213.007	-12.843
6	4	11	17.856	*	9.659	7.582	5.984
6	4	12	112.299		110.542	-108.577	-20.752
6	4	13	23.988		20.694	10.352	-17.919
6	6	0	166.634		171.992	-167.266	40.042
6	6	1	63.255		71.555	30.188	-64.875
6	6	2	135.776		144.037	-143.446	-13.036
6	6	3	17.719		12.658	-4.256	-11.921

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
6	6	4	107.516		123.803	-118.053	37.291
6	6	5	143.859		135.858	-135.424	-10.847
6	6	6	83.179		99.239	-99.100	-5.258
6	6	7	114.309		116.472	-116.032	10.111
6	6	8	0.0	*	17.217	-10.119	13.930
6	6	9	130.659		135.427	-116.309	-69.375
6	6	10	19.797	*	21.989	20.630	-7.609
6	6	11	96.377		99.917	-98.439	17.121
6	6	12	13.516	*	27.073	-24.412	11.706
6	6	13	131.971		132.444	-127.273	-36.647
6	8	0	30.639		29.350	28.592	6.628
6	8	1	191.485		207.401	-198.722	59.369
6	8	2	64.652		57.441	-54.338	-18.623
6	8	3	119.897		128.357	-119.908	-45.799
6	8	4	50.197		36.964	-36.618	5.040
6	8	5	54.796		67.539	-67.183	-6.928
6	8	6	70.274		65.976	-47.812	-45.463
6	8	7	36.792		40.834	-26.094	-31.409
6	8	8	95.469		96.123	-95.312	12.462
6	8	9	56.306		65.338	-62.456	19.194
6	8	10	103.787		107.887	-107.044	-13.461
6	8	11	26.472		20.502	-18.670	-8.469
6	10	0	135.951		130.312	-118.498	-54.217
6	10	1	42.047		35.289	3.455	-35.119
6	10	2	80.636		89.262	-88.425	-12.199
6	10	3	24.508		10.346	-9.407	4.307
6	10	4	80.119		87.093	-86.254	-12.064
6	10	5	87.373		80.966	-80.481	8.843
6	10	6	46.124		57.454	-56.010	-12.797
6	10	7	94.124		92.218	-87.077	30.362
6	10	8	39.376		47.275	-37.186	-29.192
6	10	9	67.255		68.545	-63.387	-26.088
6	10	10	41.398		41.620	14.675	-38.947
6	12	0	24.206		30.630	-30.522	-2.579
6	12	1	116.177		117.293	-104.862	52.551
6	12	2	65.611		56.564	-51.830	22.653
6	12	3	63.420		70.261	-65.907	-24.349
6	12	4	69.894		62.220	-59.811	-17.144
6	12	5	33.759		42.656	-41.897	8.009
6	12	6	53.775		45.686	-45.458	-4.552
6	12	7	48.296		49.518	-17.052	-46.490
6	14	0	78.621		69.423	-68.313	-12.364
6	14	1	43.216		43.875	-21.198	-38.414
6	14	2	45.847		42.535	-42.256	4.871
7	13	0	32.409		19.877	-12.066	-15.796
7	13	1	42.416		38.497	-32.485	20.657
7	13	2	47.388		36.118	-5.572	-35.686
7	13	3	54.617		47.748	-2.895	47.660
7	13	4	48.414		50.604	-39.796	-31.257
7	11	0	47.311		55.657	-54.156	12.841
7	11	1	102.063		92.827	-66.809	-64.448
7	11	2	25.873		23.055	-20.619	10.315
7	11	3	60.399		60.127	-38.820	-45.917

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
7	11	4	39.124		37.044	-17.631	32.579
7	11	5	42.184		47.659	-12.306	-46.043
7	11	6	48.592		49.924	0.789	49.918
7	11	7	16.202	*	31.651	-31.239	-5.094
7	9	0	56.884		40.099	-40.097	-0.437
7	9	1	26.325		12.925	6.663	11.075
7	9	2	59.036		50.682	-31.038	-40.066
7	9	3	77.787		75.324	-51.286	55.168
7	9	4	76.518		74.524	-66.837	-32.963
7	9	5	17.407	*	13.528	-6.400	-11.918
7	9	6	75.068		86.554	-30.570	-80.975
7	9	7	40.882		39.771	-32.909	22.332
7	9	8	43.392		19.811	-8.650	17.823
7	9	9	29.931		24.207	9.861	-22.107
7	9	10	39.469		33.061	-8.923	31.834
7	7	0	87.660		97.116	-96.557	10.407
7	7	1	37.010		23.865	-16.727	-17.022
7	7	2	59.851		63.044	-57.051	26.829
7	7	3	119.531		120.404	-38.572	-114.059
7	7	4	80.132		82.583	-34.729	74.926
7	7	5	22.396		16.137	8.798	-13.528
7	7	6	71.760		76.278	-23.992	72.407
7	7	8	46.690		42.936	-40.259	-14.923
7	7	9	25.188		5.122	5.116	-0.235
7	7	10	52.349		56.234	-37.011	-42.338
7	7	11	36.798		38.103	3.195	37.969
7	5	1	121.199		122.132	-60.200	106.264
7	5	2	120.350		103.909	-19.061	-102.146
7	5	3	106.720		110.755	-62.715	91.288
7	5	4	56.671		60.960	-22.776	-56.545
7	5	5	56.302		66.124	-48.425	45.027
7	5	6	128.347		136.227	-39.171	-130.474
7	5	7	45.367		50.342	-26.841	42.590
7	5	8	32.062		35.039	15.061	31.637
7	5	9	30.958		23.876	-21.081	11.210
7	5	10	0.0	*	7.763	-6.525	4.207
7	5	11	28.799		33.156	-30.349	-13.352
7	5	12	38.505		45.821	-0.469	45.818
7	3	0	33.466		47.510	-45.361	-14.129
7	3	1	142.450		139.018	-107.788	-87.794
7	3	2	119.585		119.164	-61.359	102.152
7	3	3	191.735		195.890	-36.782	-192.406
7	3	4	98.830		101.082	-14.082	100.096
7	3	5	85.357		87.927	-69.183	-54.267
7	3	6	113.495		117.190	-42.087	109.372
7	3	7	71.438		77.772	-23.036	-74.283
7	3	8	29.660		30.375	-14.871	-26.485
7	3	9	55.476		53.998	-50.727	-18.508
7	3	10	26.652		24.498	-9.851	-22.431
7	3	11	22.923		19.967	-6.171	18.989
7	3	12	64.243		60.709	-4.031	-60.575
7	3	13	71.869		74.747	-26.158	70.020
7	1	0	39.292		32.443	-28.429	15.632

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F (OBS)		F (CALC)	A (CALC)	B (CALC)
7	1	1	51.788		55.776	-42.963	35.568
7	1	2	126.159		123.285	-87.382	-86.969
7	1	3	142.334		151.132	-66.362	135.783
7	1	4	93.784		96.958	-12.744	-96.117
7	1	5	74.618		67.022	-65.407	14.626
7	1	6	136.391		129.855	-34.016	-125.321
7	1	7	51.582		43.887	0.771	43.880
7	1	8	67.558		58.509	-37.693	44.750
7	1	9	60.124		45.204	-38.182	-24.197
7	1	10	17.810	*	33.983	-15.861	30.055
7	1	11	39.887		48.772	26.574	-40.897
7	1	12	74.274		78.200	-48.034	61.709
7	1	13	93.725		102.798	-1.352	-102.789
8	0	0	94.873		89.152	89.127	2.138
8	0	1	117.850		103.658	103.441	6.703
8	0	2	121.810		116.069	115.735	8.793
8	0	3	28.670		13.321	13.094	2.453
8	0	4	244.377		219.956	219.115	19.207
8	0	5	21.485		19.042	19.025	-0.810
8	0	6	187.903		172.137	170.801	21.411
8	0	7	17.968	*	16.665	-15.969	-4.765
8	0	8	202.673		185.132	184.223	18.327
8	0	9	40.127		24.359	-23.940	-4.500
8	0	10	118.537		105.833	104.851	14.388
8	0	11	10.316	*	26.995	26.741	3.698
8	0	12	108.522		93.354	92.712	10.928
8	2	0	157.043		162.215	160.098	26.119
8	2	1	126.096		122.237	114.914	41.676
8	2	2	60.742		79.782	69.986	-38.303
8	2	3	99.931		97.510	95.467	19.857
8	2	4	30.768		37.625	37.393	-4.175
8	2	5	124.701		127.794	124.470	28.957
8	2	6	32.580		20.541	-16.995	11.538
8	2	7	147.957		150.886	150.373	12.427
8	2	8	27.280		26.601	12.708	-23.369
8	2	9	162.146		144.143	141.947	25.069
8	2	10	28.308		36.419	35.513	8.071
8	2	11	94.075		80.467	75.872	26.803
8	2	12	52.503		45.506	39.112	-23.261
8	4	0	30.768		19.221	16.649	9.604
8	4	1	51.179		67.350	66.098	-12.924
8	4	2	36.965		36.094	23.760	27.171
8	4	3	81.012		86.279	85.840	8.693
8	4	4	120.387		126.540	126.537	0.866
8	4	5	28.818		29.209	14.557	-25.324
8	4	6	143.226		151.737	147.486	35.665
8	4	7	29.713		26.969	12.668	23.809
8	4	8	91.561		103.137	102.344	-12.772
8	4	9	25.423		28.354	-24.171	-14.822
8	4	10	95.185		95.453	80.299	51.608
8	4	11	56.291		64.503	64.192	6.332
8	4	12	38.227		44.039	40.787	-16.610
8	6	0	132.614		132.852	120.397	56.163

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
8	6	1	80.222		72.785	55.140	-47.511
8	6	2	75.401		86.069	85.190	-12.271
8	6	3	119.943		111.920	106.238	35.208
8	6	4	61.063		58.768	8.172	58.197
8	6	5	98.153		98.712	89.908	-40.749
8	6	6	14.799	*	5.532	-0.113	5.531
8	6	7	136.115		143.503	142.035	20.477
8	6	8	31.582		29.373	-1.642	29.327
8	6	9	102.459		115.411	113.690	-19.858
8	6	10	54.199		49.959	49.840	3.441
8	6	11	62.134		66.105	65.690	7.389
8	8	0	68.896		40.870	38.990	-12.251
8	8	1	23.616		28.739	28.693	1.625
8	8	2	91.080		77.124	75.927	13.538
8	8	3	48.749		54.593	50.971	19.552
8	8	4	116.668		113.770	112.357	-17.875
8	8	5	33.760		38.205	18.945	-33.177
8	8	6	129.765		130.923	130.654	8.384
8	8	7	36.287		31.271	2.068	31.203
8	8	8	98.622		99.420	99.254	-5.739
8	8	9	11.448	*	10.157	-5.884	-8.280
8	10	0	58.759		67.303	66.273	11.7 3
8	10	1	88.437		69.688	66.788	19.895
8	10	2	74.890		96.233	78.554	-55.589
8	10	3	69.990		62.938	62.921	1.440
8	10	4	38.839		32.449	0.686	32.442
8	10	5	98.603		88.422	80.736	36.056
8	10	6	23.728		15.894	6.204	-14.634
8	10	7	80.528		85.374	85.167	-5.947
8	12	0	0.0	*	8.707	3.610	7.924
8	12	1	55.170		56.968	40.025	40.538
8	12	2	54.103		39.838	25.097	30.939
8	12	3	24.143		41.947	38.375	-16.938
8	12	4	59.105		53.519	51.394	-14.930
9	11	0	56.268		52.002	10.706	-50.888
9	11	1	8.506	*	18.316	17.168	6.382
9	11	2	56.684		47.385	47.384	0.316
9	11	3	48.043		51.480	5.804	51.152
9	11	4	38.227		43.936	43.914	-1.386
9	11	5	35.616		38.134	37.187	-8.446
9	9	0	124.792		120.136	74.997	93.852
9	9	1	79.464		74.559	65.514	-35.595
9	9	2	55.232		53.873	18.629	50.550
9	9	3	41.327		51.666	28.554	-43.058
9	9	4	39.672		38.732	37.345	10.275
9	9	5	42.205		38.625	35.157	-15.996
9	9	6	0.0	*	11.265	-8.259	7.661
9	9	7	26.197		33.646	24.688	22.859
9	7	0	87.314		83.526	44.307	-70.806
9	7	1	83.074		81.755	69.490	43.069
9	7	2	48.162		62.865	12.903	-61.526
9	7	3	94.528		105.951	40.723	97.812
							11.755

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CAIC)	B(CAIC)
9	7	5	67.049		66.879	66.083	10.290
9	7	6	43.361		30.991	23.587	20.102
9	7	7	17.928	*	28.824	28.771	-1.744
9	7	8	38.480		29.109	20.941	20.219
9	7	9	69.455		64.136	20.820	-60.663
9	5	0	167.829		168.718	76.181	150.540
9	5	1	59.765		58.713	58.632	3.090
9	5	2	71.694		78.793	76.736	17.884
9	5	3	61.127		66.660	49.435	-44.719
9	5	4	46.119		55.546	49.612	24.981
9	5	5	33.508		26.338	19.384	17.832
9	5	6	32.163		41.410	30.108	-28.429
9	5	7	41.661		50.884	37.038	34.890
9	5	8	55.837		53.599	51.486	-14.900
9	5	9	93.483		95.039	18.050	93.309
9	5	10	51.392		57.297	28.728	-49.575
9	3	0	127.002		130.961	61.966	-115.373
9	3	1	21.539		37.986	30.057	23.228
9	3	2	90.464		89.393	75.447	-47.947
9	3	3	90.964		90.244	46.810	77.155
9	3	4	50.837		48.662	48.658	-0.602
9	3	5	20.740		26.652	12.325	-23.631
9	3	6	78.939		78.286	69.778	35.494
9	3	7	42.934		39.833	37.159	-14.348
9	3	8	33.254		37.878	12.257	35.840
9	3	9	125.324		116.417	16.762	-115.205
9	3	10	82.730		77.404	30.639	71.082
9	3	11	45.581		42.343	10.777	-40.948
9	1	0	184.733		176.189	74.526	159.651
9	1	1	57.042		60.342	52.261	-30.165
9	1	2	82.168		79.753	27.017	75.038
9	1	3	150.260		146.210	107.304	-99.314
9	1	4	48.359		44.395	27.049	35.203
9	1	5	52.664		41.484	39.398	-12.991
9	1	6	60.561		56.101	53.991	-15.242
9	1	7	44.930		43.953	41.701	13.887
9	1	8	10.038	*	23.016	8.885	-21.232
9	1	9	111.161		105.145	22.092	102.798
9	1	10	88.549		83.067	56.712	-60.695
9	1	11	41.589		28.956	10.982	26.793
10	0	0	72.022		65.274	-64.293	-11.274
10	0	1	43.685		31.142	-31.117	-1.236
10	0	2	162.979		153.769	-153.019	-15.176
10	0	3	53.745		45.425	45.222	4.291
10	0	4	64.299		59.296	-57.797	-13.248
10	0	5	26.559	*	18.953	18.713	3.005
10	0	6	125.598		104.946	-104.107	-13.241
10	0	7	52.948		53.008	-52.804	-4.655
10	0	8	83.810		66.747	-66.083	-9.395
10	0	9	65.944		78.124	-77.471	-10.080
10	0	10	28.796		20.343	-20.300	-1.329
10	2	0	43.581		34.066	22.584	-25.504
10	2	1	114.024		121.187	-121.187	-0.194

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
10	2	2	24.633		23.486	23.485	-0.196
10	2	3	135.779		144.671	-144.660	1.790
10	2	4	50.233		38.260	-28.712	-25.287
10	2	5	158.378		165.425	-164.868	13.554
10	2	6	26.082		8.463	6.155	5.809
10	2	7	44.121		47.734	-45.951	-12.922
10	2	8	38.537		38.797	-24.439	-30.132
10	2	9	47.940		44.767	-42.925	12.712
10	2	10	60.333		64.858	-64.669	-4.939
10	4	0	144.208		131.398	-131.308	4.850
10	4	1	40.250		27.888	-11.864	-25.239
10	4	2	158.927		155.265	-154.312	17.183
10	4	3	51.118		49.158	46.494	15.961
10	4	4	112.391		120.647	-114.816	-37.054
10	4	5	42.706		47.061	44.748	-14.573
10	4	6	108.553		117.984	-117.981	0.796
10	4	7	56.312		57.092	-56.955	3.962
10	4	8	95.926		103.087	-102.789	-7.832
10	4	9	44.199		43.574	-43.292	4.948
10	4	10	34.453		29.019	-28.537	5.270
10	6	0	31.872		22.172	-14.692	-16.606
10	6	1	115.364		108.785	-105.634	-25.992
10	6	2	44.861		38.927	32.555	21.342
10	6	3	125.080		121.555	-121.463	-4.744
10	6	4	39.029		41.060	-41.059	-0.208
10	6	5	119.673		122.626	-122.535	-4.736
10	6	6	31.900		47.133	9.445	46.177
10	6	7	49.660		58.141	-48.277	-32.399
10	6	8	44.768		41.408	-27.667	-30.809
10	6	9	8.979	*	33.239	-32.777	-5.521
10	8	0	110.166		90.281	-88.033	20.021
10	8	1	32.461		26.889	-14.549	-22.613
10	8	2	84.490		73.909	-73.858	-2.764
10	8	3	0.0	*	16.588	4.264	16.031
10	8	4	55.251		60.451	-52.839	-29.365
10	8	5	31.104		30.834	-0.931	-30.820
10	8	6	59.511		62.350	-60.884	-13.443
10	8	7	50.102		57.037	-53.744	19.100
10	10	0	41.916		22.941	-8.717	-21.221
10	10	1	58.160		58.363	-58.159	4.884
10	10	2	26.147		20.754	2.713	-20.576
10	10	3	87.847		90.214	-89.529	11.093
10	10	4	32.826		26.632	-26.347	-3.887
10	10	5	66.708		75.138	-69.706	28.050
10	12	0	87.922		76.236	-67.488	35.459
11	11	0	53.280		44.642	-41.268	-17.026
11	11	1	55.208		65.737	-59.492	-27.965
11	9	0	37.648		39.904	-33.908	-21.037
11	9	1	11.098	*	11.650	-11.531	-1.661
11	9	2	55.820		54.849	-54.111	8.970
11	9	3	79.919		71.720	-53.120	-48.188
11	9	4	46.187		50.997	-49.390	-12.699
11	7	0	63.966		60.835	-59.233	13.871

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
11	7	1	56.124		76.921	-63.850	-42.894
11	7	2	74.848		53.319	-51.015	-15.507
11	7	3	56.384		52.878	-2.087	52.836
11	7	4	28.168		27.002	-24.943	-10.340
11	7	5	63.064		63.597	-40.993	48.623
11	7	6	93.807		91.829	-52.043	-75.658
11	5	0	7.885	*	23.167	-11.993	-19.821
11	5	1	54.820		51.969	-47.949	20.042
11	5	2	62.590		66.559	-66.559	0.169
11	5	3	83.291		77.382	-66.731	-39.178
11	5	4	32.917		39.065	-33.494	-20.104
11	5	5	74.804		74.184	-36.645	-64.501
11	5	6	77.691		73.675	-34.120	65.298
11	5	7	31.497		40.987	-38.428	-14.255
11	5	8	41.969		45.353	-11.187	43.952
11	3	0	85.988		77.686	-71.940	29.322
11	3	1	103.269		114.255	-83.901	-77.557
11	3	2	49.790		42.688	-39.329	-16.598
11	3	3	69.357		70.716	-53.893	45.785
11	3	4	37.350		35.627	-35.274	-5.003
11	3	5	80.726		75.878	-53.920	53.386
11	3	6	92.980		91.108	-26.070	-87.298
11	3	7	61.781		64.404	-63.820	8.653
11	3	8	72.606		77.407	-29.953	-71.377
11	3	9	37.853		38.863	-31.926	22.159
11	1	0	94.675		99.864	-92.676	-37.202
11	1	1	76.434		71.799	-64.872	30.770
11	1	2	19.294		23.847	-20.291	12.528
11	1	3	104.986		96.606	-46.157	-84.866
11	1	4	96.046		102.827	-102.705	-5.016
11	1	5	101.345		95.540	-16.421	-94.118
11	1	6	119.093		109.476	-33.284	104.293
11	1	7	64.995		56.724	-30.740	-47.673
11	1	8	97.738		87.125	-65.145	57.852
11	1	9	50.393		45.077	0.546	-45.073
12	0	0	90.829		85.767	84.731	13.292
12	0	1	46.281		45.089	-44.590	-6.686
12	0	2	177.386		159.393	158.627	15.606
12	0	3	22.628		18.100	18.088	-0.651
12	0	4	95.174		82.633	81.943	10.651
12	0	5	32.836		39.547	39.365	3.783
12	0	6	61.326		48.175	48.071	3.178
12	0	7	33.585		31.349	30.572	6.938
12	0	8	14.935	*	27.361	-27.219	-2.787
12	2	0	22.311		30.348	17.133	-25.048
12	2	1	96.889		88.138	79.038	39.004
12	2	2	49.254		44.319	-41.869	14.533
12	2	3	67.001		64.775	64.482	-6.153
12	2	4	22.637		19.838	12.174	-15.663
12	2	5	46.188		36.926	29.240	22.551
12	2	6	46.075		53.763	53.763	-0.099
12	2	7	50.658		37.393	36.716	7.084
12	2	8	113.812		113.374	113.251	-5.277

JCAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
12	4	0	35.785		34.625	34.143	5.758
12	4	1	0.0	*	10.631	-8.563	6.300
12	4	2	113.429		118.900	118.120	13.599
12	4	3	34.837		28.391	8.215	-27.177
12	4	4	33.017		46.398	45.910	-6.709
12	4	5	67.351		62.122	55.587	27.736
12	4	6	25.327		19.906	14.061	14.090
12	4	7	46.315		44.382	42.554	-12.606
12	6	0	25.167		27.755	11.196	-25.396
12	6	1	87.810		89.394	87.765	-16.993
12	6	2	46.684		51.324	-28.823	42.466
12	6	3	43.024		46.802	46.728	2.629
12	6	4	0.0	*	10.313	3.290	9.774
12	6	5	25.525		36.268	36.078	-3.711
12	6	6	45.694		46.477	46.058	6.227
12	8	0	36.985		36.842	36.746	2.654
12	8	1	8.208	*	11.593	-8.628	-7.743
12	8	2	91.740		94.935	94.221	-11.622
12	8	3	26.021		21.124	8.147	-19.490
12	8	4	56.730		65.812	65.046	-10.011
12	10	0	37.348		32.319	20.681	-24.836
12	10	1	70.640		68.291	68.290	0.447
13	9	0	29.962		29.773	29.442	4.431
13	7	0	63.429		50.921	49.813	10.565
13	7	1	51.816		53.860	52.653	-11.339
13	7	2	79.369		68.421	30.213	61.389
13	7	3	61.617		59.742	56.725	-18.746
13	5	0	59.492		56.908	52.502	-21.955
13	5	1	63.416		49.503	20.767	44.937
13	5	2	65.355		68.961	56.512	-39.523
13	5	3	75.042		68.114	48.333	47.994
13	5	4	68.081		71.885	44.544	-56.420
13	5	5	52.932		53.447	22.528	48.467
13	3	0	72.830		63.710	56.554	29.337
13	3	1	62.621		67.984	51.120	-44.817
13	3	2	91.288		88.696	48.101	74.520
13	3	3	57.064		56.950	35.358	-44.644
13	3	4	88.487		89.945	53.188	72.533
13	3	5	64.356		63.332	43.741	-45.801
13	3	6	39.079		42.181	20.657	36.777
13	1	0	29.074		35.293	32.961	-12.617
13	1	1	91.020		85.961	81.080	28.555
13	1	2	85.329		86.008	68.321	-52.246
13	1	3	42.082		46.330	13.675	44.266
13	1	4	74.512		68.324	44.625	-51.738
13	1	5	71.248		75.930	61.189	44.958
13	1	6	61.569		50.606	41.587	-28.836
14	0	0	65.944		54.596	-54.142	-7.020
14	0	1	49.639		38.792	-38.752	-1.776
14	0	2	25.267		23.738	23.726	0.774
14	0	3	16.686	*	13.476	-12.341	-5.415
14	0	4	0.0	*	19.328	18.950	3.804
14	2	0	7.641	*	12.589	11.080	-5.977

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
14	2	1	17.667	*	18.134	-14.818	10.454
14	2	2	49.759		46.358	-42.328	-18.903
14	2	3	40.154		40.464	-40.228	4.362
14	2	4	59.428		58.976	-58.969	-0.853
14	4	0	70.162		72.205	-72.157	2.623
14	4	1	29.798		21.698	-11.777	18.223
14	4	2	19.516		19.394	-17.486	-8.388
14	4	3	15.264	*	21.615	-14.992	-15.570
14	6	0	10.540	*	15.783	15.016	4.862
14	6	1	12.615	*	13.653	-9.113	10.166
14	6	2	57.405		50.708	-48.625	14.382
15	5	0	44.659		36.899	-23.838	28.165
15	3	0	74.081		69.871	-32.451	-61.878
15	3	1	75.772		69.482	-45.644	52.387
15	3	2	44.494		39.802	-33.848	-20.941
15	1	0	81.566		76.706	-54.619	53.857
15	1	1	93.697		85.749	-15.918	-84.259
15	1	2	74.686		74.100	-69.799	24.878
16	0	0	38.528		22.896	22.879	-0.896
-16	4	10	30.358		28.892	-25.979	12.643
-16	4	9	42.093		45.544	-43.136	-14.613
-16	4	8	42.166		44.123	44.047	2.585
-16	4	7	23.960		20.665	-20.282	3.962
-16	4	6	40.668		35.571	34.826	-7.240
-16	4	5	29.670		32.918	-15.987	-28.775
-16	4	4	40.499		34.093	32.829	9.194
-16	4	3	41.965		26.818	-24.830	10.133
-16	2	11	27.566		25.771	24.696	7.365
-16	2	10	23.224		24.458	16.569	-17.990
-16	2	9	39.272		49.134	49.082	2.260
-16	2	8	61.498		74.019	-72.648	-14.179
-16	2	7	26.633		34.290	26.377	21.910
-16	2	6	34.054		40.923	-39.493	-10.723
-16	2	5	5.457	*	12.753	12.751	0.223
-16	2	4	40.262		42.509	-40.866	-11.702
-16	2	3	41.948		47.536	45.905	12.344
-16	2	2	57.685		49.238	49.188	-2.214
-16	2	1	17.988	*	10.763	9.829	-4.386
-16	0	12	28.050		13.807	13.801	0.374
-16	0	11	55.869		50.462	-50.095	-6.075
-16	0	10	15.706	*	7.833	7.278	2.909
-16	0	9	70.937		62.389	-61.788	-8.634
-16	0	8	66.489		65.180	64.647	8.318
-16	0	7	42.262		42.985	-42.280	-7.755
-16	0	6	75.592		85.552	84.947	10.157
-16	0	5	21.519		23.533	-22.687	-6.253
-16	0	4	54.344		57.043	56.665	6.558
-16	0	3	38.796		40.512	-40.240	-4.690
-16	0	2	20.459	*	15.231	-15.224	0.463
-16	0	1	33.092		5.306	-5.246	0.796
-15	1	14	53.155		46.337	-30.899	-34.531
-15	1	13	46.742		40.290	-39.889	5.675
-15	1	12	80.269		77.548	-47.919	-60.970

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-15	1	11	66.255		62.423	-44.510	43.767
-15	1	10	31.723		40.869	-32.739	-24.464
-15	1	9	70.776		82.291	-62.179	53.905
-15	1	8	62.855		70.345	-58.521	-39.034
-15	1	7	29.531		31.531	-26.911	-16.432
-15	1	6	47.363		45.646	-39.555	-22.781
-15	1	5	61.130		76.420	-71.510	-26.948
-15	1	4	55.915		63.872	-63.855	1.464
-15	1	3	24.620		38.094	-20.207	-32.293
-15	1	2	72.294		81.646	-56.619	58.825
-15	1	1	59.597		68.847	-51.594	-45.585
-15	3	13	41.503		42.679	-36.801	-21.614
-15	3	12	64.090		62.061	-45.806	41.873
-15	3	11	87.595		95.634	-43.621	-85.106
-15	3	10	48.730		52.674	-35.783	38.655
-15	3	9	83.868		92.637	-58.421	-71.893
-15	3	8	57.430		55.775	-51.652	21.044
-15	3	7	57.988		70.594	-59.201	-38.454
-15	3	6	45.731		48.795	-30.153	38.363
-15	3	5	62.094		64.039	-63.907	4.119
-15	3	4	38.617		44.658	-38.468	-22.683
-15	3	3	46.260		46.112	-46.028	-2.784
-15	3	2	80.745		74.585	-46.876	-58.014
-15	3	1	79.146		74.261	-73.210	12.446
-15	5	11	81.904		81.997	-70.708	41.519
-15	5	10	39.666		42.404	-28.047	-31.804
-15	5	9	71.753		68.694	-19.410	65.895
-15	5	8	48.419		50.116	-28.074	-41.514
-15	5	7	71.585		70.549	-70.527	1.762
-15	5	6	55.956		60.005	-53.249	-27.662
-15	5	5	31.601		31.207	-27.494	-14.764
-15	5	4	37.332		41.162	-41.018	-3.429
-15	5	3	68.303		63.551	-62.142	-13.307
-15	5	2	67.875		68.801	-44.214	52.714
-15	5	1	39.179		36.937	-24.201	-27.904
-15	7	8	56.815		56.338	-52.642	20.070
-15	7	7	37.689		29.274	-29.110	-3.095
-15	7	6	46.206		37.976	-28.902	24.634
-15	7	5	40.181		35.196	-34.793	5.312
-15	7	4	50.802		47.459	-42.033	-22.035
-15	7	3	38.327		38.437	-35.295	15.221
-14	8	9	29.238		29.617	-20.233	21.629
-14	8	8	0.0	*	20.404	-19.076	-7.240
-14	8	7	0.0	*	10.395	7.452	7.247
-14	8	6	9.327	*	0.874	-0.858	-0.166
-14	8	5	33.556		31.839	31.627	-3.669
-14	8	4	46.155		42.663	-39.665	-15.711
-14	8	3	14.595	*	15.277	12.270	9.101
-14	8	2	55.498		53.656	-50.939	16.858
-14	8	1	21.567		3.278	-1.519	-2.905
-14	6	12	41.192		37.831	-34.895	14.613
-14	6	11	45.959		43.031	41.141	-12.612
-14	6	10	33.623		31.416	-4.316	31.118

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-14	6	9	0.0	*	13.912	-6.156	-12.476
-14	6	8	14.390	*	10.800	8.676	6.432
-14	6	7	13.166	*	14.447	-10.717	-9.687
-14	6	6	38.971		39.339	2.006	39.288
-14	6	5	80.843		85.938	-85.106	-11.926
-14	6	4	34.355		30.931	30.742	3.413
-14	6	3	38.394		37.386	-33.126	17.331
-14	6	2	42.753		39.248	37.207	12.491
-14	6	1	81.531		71.898	-66.532	-27.256
-14	4	14	63.845		62.048	61.678	6.769
-14	4	13	16.909	*	10.415	-9.559	4.134
-14	4	12	28.855		22.360	22.157	3.005
-14	4	11	49.052		47.588	-47.353	-4.724
-14	4	10	24.444		19.933	1.851	19.847
-14	4	9	0.0	*	4.040	3.516	1.988
-14	4	8	49.002		51.359	-51.018	-5.911
-14	4	7	17.195	*	13.248	2.732	12.963
-14	4	6	22.409		24.256	-22.957	7.832
-14	4	5	65.466		68.486	68.466	-1.658
-14	4	4	90.514		92.103	-90.882	-14.949
-14	4	3	32.675		26.336	21.830	14.732
-14	4	2	85.928		86.007	-85.248	11.401
-14	4	1	41.422		33.132	30.826	-12.147
-14	2	15	53.525		51.848	51.495	6.045
-14	2	14	90.680		84.716	-83.734	-12.862
-14	2	13	31.884		33.273	29.205	15.943
-14	2	12	16.701	*	14.567	-14.428	-2.004
-14	2	11	30.433		37.271	35.748	10.546
-14	2	10	24.677		29.841	-27.667	-11.182
-14	2	9	0.0	*	13.809	6.483	12.192
-14	2	8	35.951		28.322	28.052	-3.904
-14	2	7	36.652		35.798	-35.784	-0.973
-14	2	6	13.763	*	13.092	10.303	8.077
-14	2	5	82.731		93.192	-93.102	-4.101
-14	2	4	43.416		45.111	45.107	0.618
-14	2	3	46.667		54.779	-54.376	6.629
-14	2	2	49.219		47.018	46.080	-9.345
-14	2	1	78.386		70.638	-70.388	5.938
-14	0	15	51.467		47.712	-47.073	-7.783
-14	0	14	81.373		82.691	81.921	11.259
-14	0	13	18.528	*	18.892	-17.810	-6.303
-14	0	12	61.663		66.850	66.182	9.427
-14	0	11	79.925		83.244	-82.883	-7.749
-14	0	10	31.815		41.507	41.396	3.030
-14	0	9	18.895		4.184	2.012	-3.668
-14	0	8	15.818	*	9.671	-9.371	-2.387
-14	0	7	20.060	*	24.213	-24.153	1.704
-14	0	6	17.898	*	6.457	-4.890	-4.216
-14	0	5	90.031		90.021	89.688	7.735
-14	0	4	72.865		76.652	-76.143	-8.820
-14	0	3	18.487	*	7.564	6.145	4.410
-14	0	2	44.299		48.931	-47.814	-10.396
-14	0	1	27.500		31.906	31.858	1.763

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
-13	1	16	55.913	51.774	45.836	-24.076
-13	1	15	48.540	48.108	38.194	29.250
-13	1	14	55.542	58.872	49.414	-32.003
-13	1	13	73.682	60.715	60.512	-4.968
-13	1	12	31.063	45.808	41.121	20.184
-13	1	11	69.751	64.826	55.473	-33.543
-13	1	10	73.717	75.904	60.403	45.966
-13	1	9	86.330	83.739	81.102	-20.849
-13	1	8	82.811	91.083	31.208	85.570
-13	1	7	99.898	100.517	64.196	-77.346
-13	1	6	93.812	96.102	70.793	64.992
-13	1	5	93.653	106.506	77.402	-73.160
-13	1	4	42.534	54.215	26.235	47.445
-13	1	3	72.854	93.920	85.846	-38.096
-13	1	2	67.476	77.608	72.352	28.075
-13	1	1	48.263	60.838	41.350	44.625
-13	3	16	76.652	76.208	48.395	58.869
-13	3	15	47.519	51.307	37.000	-35.544
-13	3	14	41.457	51.995	46.449	23.367
-13	3	13	40.764	39.010	38.202	-7.903
-13	3	12	89.507	94.456	81.260	48.152
-13	3	11	31.545	25.845	23.940	9.740
-13	3	10	74.331	74.920	54.895	-50.985
-13	3	9	52.258	48.712	46.291	15.166
-13	3	8	82.459	81.036	72.615	-35.972
-13	3	7	74.333	75.881	44.121	61.736
-13	3	6	86.492	89.655	69.806	-56.259
-13	3	5	77.963	90.047	54.935	71.348
-13	3	4	57.907	65.171	61.580	-21.332
-13	3	3	54.787	47.337	43.546	18.561
-13	3	2	59.202	63.561	63.275	6.013
-13	3	1	61.703	64.071	44.029	-46.546
-13	5	15	63.909	66.497	44.771	49.167
-13	5	14	58.868	53.885	40.151	-35.937
-13	5	13	32.518	37.870	36.582	9.795
-13	5	12	55.956	48.243	48.018	4.657
-13	5	11	57.439	57.191	56.016	-11.535
-13	5	10	81.272	67.799	60.352	30.891
-13	5	9	56.983	60.330	59.176	11.744
-13	5	8	97.847	92.568	58.121	72.048
-13	5	7	86.728	78.277	47.060	-62.551
-13	5	6	89.681	77.806	60.351	49.107
-13	5	5	63.464	61.987	57.387	-23.433
-13	5	4	60.375	55.678	50.660	23.100
-13	5	3	51.750	43.944	39.217	-19.826
-13	5	2	100.864	87.451	85.486	18.436
-13	5	1	75.557	90.504	59.954	67.797
-13	7	13	58.784	53.679	52.977	8.650
-13	7	12	77.335	69.991	65.649	24.267
-13	7	11	57.429	52.507	43.913	28.786
-13	7	10	34.353	35.332	16.271	-31.362
-13	7	9	74.265	64.523	48.273	42.813
-13	7	8	85.102	80.293	66.805	-44.544

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-13	7	7	69.111		70.836	53.198	46.774
-13	7	6	45.906		42.079	29.300	-30.202
-13	7	5	124.128		112.153	73.237	84.939
-13	7	4	78.260		70.644	69.371	-13.353
-13	7	3	70.028		59.681	50.553	31.721
-13	7	2	11.957	*	8.174	6.974	-4.265
-13	7	1	60.056		60.154	59.705	-7.337
-13	9	10	61.691		60.471	47.725	37.136
-13	9	9	59.392		58.983	58.391	-8.334
-13	9	8	64.952		61.463	32.490	52.174
-13	9	7	70.325		56.435	40.894	-38.892
-13	9	6	64.628		58.472	40.934	41.754
-13	9	5	56.856		46.387	30.999	-34.508
-13	9	4	45.467		37.029	34.966	12.187
-13	9	3	58.118		46.608	41.485	-21.243
-13	9	2	76.271		61.184	51.839	32.499
-13	9	1	62.072		61.686	58.434	19.766
-12	10	10	61.485		56.155	45.246	-33.259
-12	10	9	21.186		12.583	-10.364	-7.135
-12	10	8	65.725		59.511	55.215	-22.200
-12	10	7	9.567	*	10.404	10.402	-0.205
-12	10	6	40.050		32.767	25.968	-19.983
-12	10	5	33.688		30.204	9.244	28.754
-12	10	4	9.851	*	12.880	-12.814	1.301
-12	10	3	27.862		44.089	44.038	2.122
-12	10	2	22.208		29.190	-8.083	-28.049
-12	10	1	63.402		66.929	66.779	-4.485
-12	8	13	39.038		32.273	29.206	-13.733
-12	8	12	19.254	*	16.273	-1.140	-16.233
-12	8	11	70.926		59.854	59.572	-5.803
-12	8	10	8.620	*	14.307	-7.271	-12.322
-12	8	9	24.584		21.291	20.131	6.932
-12	8	8	67.251		57.600	-54.664	18.155
-12	8	7	68.256		50.734	46.161	-21.050
-12	8	6	40.977		57.438	53.730	-20.304
-12	8	5	0.0	*	9.580	3.459	-8.933
-12	8	4	40.936		53.743	49.658	-20.552
-12	8	3	27.828		18.177	11.939	-13.706
-12	8	2	86.605		95.416	94.811	10.728
-12	8	1	53.223		46.395	-44.713	12.381
-12	6	15	27.045		35.861	-16.766	-31.700
-12	6	14	34.923		36.001	22.373	28.205
-12	6	13	18.099	*	18.589	-17.232	-6.972
-12	6	12	33.616		32.794	20.784	25.368
-12	6	11	88.673		81.393	-75.896	-29.403
-12	6	10	74.889		71.055	70.870	5.121
-12	6	9	0.0	*	8.635	8.553	1.193
-12	6	8	91.279		88.428	82.112	-32.819
-12	6	7	45.267		33.059	-26.488	-19.782
-12	6	6	57.274		47.536	24.815	40.545
-12	6	5	39.709		41.416	30.572	27.941
-12	6	4	23.116		22.258	-18.961	-11.658
-12	6	3	52.419		58.514	38.327	-44.214

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-12	6	2	42.737		37.962	-9.233	36.822
-12	6	1	106.689		107.671	107.616	3.437
-12	4	16	39.756		34.925	-33.719	9.098
-12	4	15	30.127		24.478	24.335	2.634
-12	4	14	31.049		26.545	-19.416	-18.101
-12	4	13	52.502		51.925	51.600	-5.801
-12	4	12	38.842		42.039	-41.294	-7.878
-12	4	11	99.879		92.801	92.800	0.354
-12	4	10	70.665		62.766	-62.667	-3.523
-12	4	9	59.451		53.644	53.002	8.277
-12	4	8	84.649		79.820	-78.321	15.396
-12	4	7	54.465		49.864	48.129	-13.041
-12	4	6	10.032	*	9.789	7.850	-5.848
-12	4	5	52.937		50.464	49.737	-8.532
-12	4	4	42.762		51.642	50.622	-9.697
-12	4	3	19.354		18.479	18.479	0.086
-12	4	2	73.458		76.397	69.100	32.584
-12	4	1	61.464		61.561	-59.141	-17.089
-12	2	17	27.620		34.648	33.718	-7.973
-12	2	16	41.479		27.319	26.134	-7.956
-12	2	15	13.654	*	9.945	-2.028	9.736
-12	2	14	22.993		8.171	7.777	-2.507
-12	2	13	57.601		54.205	-54.204	0.314
-12	2	12	79.903		63.128	63.052	3.109
-12	2	11	87.114		80.098	-80.085	-1.453
-12	2	10	59.900		58.045	56.939	-11.278
-12	2	9	18.564		5.280	-2.187	4.806
-12	2	8	137.322		135.037	135.037	0.337
-12	2	7	40.024		36.414	-35.734	7.006
-12	2	6	0.0	*	12.947	-3.340	-12.509
-12	2	5	34.483		37.023	35.257	11.296
-12	2	4	15.114	*	5.490	3.383	-4.324
-12	2	3	33.132		42.973	29.007	31.706
-12	2	2	32.543		34.000	-27.840	-19.518
-12	2	1	148.995		156.336	156.333	-1.004
-12	0	17	68.333		81.023	-80.671	-7.549
-12	0	16	0.0	*	9.072	9.060	0.468
-12	0	15	38.748		28.345	28.343	0.398
-12	0	14	19.264		10.200	-10.009	-1.964
-12	0	13	25.341		12.247	10.324	6.587
-12	0	12	24.933		28.877	28.631	-3.758
-12	0	11	125.322		125.360	124.931	10.359
-12	0	10	63.635		67.742	-67.321	-7.542
-12	0	9	0.0	*	10.465	8.001	6.746
-12	0	8	25.526		34.487	-34.066	-5.369
-12	0	7	68.664		79.100	78.905	5.545
-12	0	6	50.294		43.325	43.254	2.486
-12	0	5	13.922	*	27.191	27.053	2.735
-12	0	4	97.012		100.763	100.289	9.756
-12	0	3	18.851		16.144	-15.783	-3.397
-12	0	2	128.895		136.987	136.412	12.541
-12	0	1	76.146		75.633	-75.114	-8.837
-11	1	17	53.613		55.843	-35.550	-43.066

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
-11	1	16	94.553	87.921	-63.606	60.699
-11	1	15	51.870	44.326	-39.126	-20.832
-11	1	14	105.480	99.896	-71.203	70.066
-11	1	13	130.727	139.788	-37.396	-134.693
-11	1	12	68.483	75.981	-73.857	17.841
-11	1	11	94.893	95.438	-65.603	-69.316
-11	1	10	92.575	96.156	-85.800	43.409
-11	1	9	52.240	52.378	-48.006	-20.947
-11	1	8	54.458	60.640	-60.202	-7.278
-11	1	7	126.811	120.364	-90.539	79.310
-11	1	6	83.560	87.218	-77.896	-39.233
-11	1	5	52.015	56.896	-56.275	-8.387
-11	1	4	145.653	157.787	-81.248	-135.261
-11	1	3	76.218	92.705	-89.581	23.864
-11	1	2	41.536	49.514	-38.916	-30.613
-11	1	1	95.981	100.117	-62.054	78.567
-11	3	17	64.664	63.443	-62.976	-7.683
-11	3	16	67.241	70.577	-43.490	-55.586
-11	3	15	66.493	70.987	-70.178	10.690
-11	3	14	87.943	87.606	-41.650	-77.073
-11	3	13	91.795	87.362	-74.713	45.279
-11	3	12	44.868	42.685	-42.128	-6.875
-11	3	11	104.365	97.067	-62.193	74.525
-11	3	10	93.812	96.826	-68.696	-68.236
-11	3	9	92.723	93.404	-74.315	-56.582
-11	3	8	83.775	79.400	-79.115	6.719
-11	3	7	119.113	127.246	-89.722	-90.231
-11	3	6	69.435	72.315	-65.566	30.507
-11	3	5	74.284	86.044	-61.735	-59.936
-11	3	4	141.114	150.059	-48.927	141.859
-11	3	3	135.111	140.059	-105.872	-91.694
-11	3	2	65.469	63.039	-55.163	30.512
-11	3	1	128.026	121.961	-61.336	-105.416
-11	5	16	44.932	41.721	-28.899	30.090
-11	5	15	34.528	24.004	-23.142	6.374
-11	5	14	81.731	72.953	-50.694	52.462
-11	5	13	141.014	129.403	-88.879	-94.052
-11	5	12	51.667	47.967	-47.904	2.452
-11	5	11	63.214	57.726	-44.429	-36.856
-11	5	10	67.657	61.527	-60.649	10.355
-11	5	9	85.395	88.248	-88.248	-0.044
-11	5	8	32.371	25.993	-20.553	15.913
-11	5	7	87.611	86.123	-49.168	70.708
-11	5	6	99.270	102.889	-62.536	-81.703
-11	5	5	99.189	101.028	-96.068	31.267
-11	5	4	113.617	111.707	-46.439	-101.597
-11	5	3	89.823	83.571	-73.829	39.159
-11	5	2	91.065	89.124	-64.530	-61.473
-11	5	1	107.123	99.688	-55.361	82.903
-11	7	15	52.650	52.853	-45.966	26.089
-11	7	14	68.995	67.608	-42.189	-52.829
-11	7	13	78.007	68.348	-26.140	63.152
-11	7	12	57.566	57.065	-54.259	-17.676

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-11	7	11	67.682		57.882	-31.210	48.747
-11	7	10	88.932		82.269	-60.288	-55.979
-11	7	9	58.942		48.204	-48.161	-2.043
-11	7	8	78.013		82.973	-82.477	9.058
-11	7	7	84.787		78.799	-56.418	-55.012
-11	7	6	70.160		75.024	-74.613	-7.840
-11	7	5	29.922		23.600	-21.317	-10.126
-11	7	4	113.283		115.278	-43.660	106.691
-11	7	3	83.860		66.880	-40.289	-53.383
-11	7	2	70.441		76.679	-76.390	6.661
-11	7	1	76.758		66.193	-45.073	-48.476
-11	9	13	107.377		96.082	-57.558	-76.934
-11	9	12	64.873		52.762	-52.317	6.842
-11	9	11	74.960		68.719	-56.597	-38.977
-11	9	10	67.283		48.283	-46.921	11.389
-11	9	9	58.990		55.158	-53.360	-13.968
-11	9	8	32.040		23.058	-22.931	2.420
-11	9	7	29.742		26.753	-20.583	17.090
-11	9	6	82.681		73.009	-67.244	-28.437
-11	9	5	83.523		80.758	-80.758	-0.170
-11	9	4	95.872		95.868	-64.381	-71.034
-11	9	3	17.519	*	25.184	-25.148	-1.332
-11	9	2	75.242		64.205	-60.810	-20.603
-11	9	1	62.701		53.119	-42.381	32.023
-11	11	9	53.664		49.643	-47.031	-15.889
-11	11	8	72.318		68.904	-66.338	-18.627
-11	11	7	81.141		81.138	-67.349	-45.249
-11	11	6	30.883		36.313	-24.963	26.372
-11	11	5	44.284		40.705	-34.491	-21.617
-11	11	4	42.990		40.145	-27.756	29.003
-11	11	3	69.765		63.583	-42.979	-46.857
-11	11	2	61.597		47.454	-37.630	28.911
-11	11	1	86.209		72.168	-59.049	-41.490
-10	12	8	33.417		36.117	-23.779	27.185
-10	12	7	55.344		47.716	-41.023	24.371
-10	12	6	20.371		8.565	-6.388	5.706
-10	12	5	39.014		31.676	-31.547	-2.859
-10	12	4	0.0	*	13.635	-13.614	0.761
-10	12	3	32.886		17.134	-15.261	-7.789
-10	12	2	25.285		39.294	-35.752	-16.303
-10	12	1	67.951		54.666	-50.541	20.833
-10	10	12	32.812		36.347	-35.630	-7.189
-10	10	11	67.506		63.374	-23.881	58.702
-10	10	10	5.027	*	34.525	-34.465	2.033
-10	10	9	47.324		49.661	43.793	-23.417
-10	10	8	60.912		54.319	-51.222	-18.080
-10	10	7	22.496		32.281	11.602	30.124
-10	10	6	56.852		56.728	-51.779	-23.175
-10	10	5	21.634		14.033	2.791	-13.753
-10	10	4	110.857		99.971	-98.371	17.818
-10	10	3	39.397		46.096	-21.558	40.745
-10	10	2	35.972		24.910	-24.872	-1.373
-10	10	1	35.314		31.996	-23.621	-21.583

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-10	8	15	0.0	*	9.006	-8.860	1.619
-10	8	14	56.649		50.817	-44.937	23.728
-10	8	13	35.476		20.107	20.020	-1.869
-10	8	12	34.868		35.431	34.863	-6.321
-10	8	11	43.619		47.447	-42.387	-21.320
-10	8	10	22.106		16.712	13.265	-10.165
-10	8	9	69.014		70.468	-69.565	11.244
-10	8	8	30.612		25.924	10.869	23.535
-10	8	7	121.324		115.451	-115.326	-5.362
-10	8	6	36.965		26.329	25.180	-7.695
-10	8	5	64.728		56.456	-51.888	22.248
-10	8	4	55.667		37.251	36.663	-6.593
-10	8	3	95.308		75.922	-63.503	-41.612
-10	8	2	29.542		41.551	-23.303	-34.402
-10	8	1	80.088		67.000	-54.673	38.727
-10	6	16	55.413		56.221	55.058	11.378
-10	6	15	37.666		36.713	-36.489	4.043
-10	6	14	40.452		32.187	31.126	-8.197
-10	6	13	44.765		39.718	-38.956	-7.740
-10	6	12	66.349		58.199	-55.439	17.711
-10	6	11	39.968		41.427	-29.447	29.138
-10	6	10	64.433		60.924	-59.453	13.306
-10	6	9	64.467		59.261	57.011	-16.173
-10	6	8	74.846		75.192	-73.762	14.595
-10	6	7	44.241		33.638	27.429	-19.472
-10	6	6	80.648		73.089	-72.987	3.862
-10	6	5	30.240		19.574	10.424	-16.568
-10	6	4	162.943		151.713	-142.176	52.941
-10	6	3	42.447		59.876	-56.066	-21.019
-10	6	2	61.404		47.817	-33.653	33.971
-10	6	1	15.935	*	17.308	-15.784	-7.102
-10	4	17	45.628		45.225	42.137	16.423
-10	4	16	95.628		95.455	-95.332	4.837
-10	4	15	16.932	*	23.346	22.285	-6.957
-10	4	14	85.594		83.791	-81.786	18.221
-10	4	13	17.844	*	20.578	19.614	6.227
-10	4	12	12.987	*	12.003	10.883	5.065
-10	4	11	17.631	*	22.697	-11.516	-19.558
-10	4	10	19.242		13.004	-9.702	-8.659
-10	4	9	119.254		115.115	-115.074	3.075
-10	4	8	38.883		37.025	9.037	35.905
-10	4	7	118.550		119.938	-116.882	-26.902
-10	4	6	21.547		32.132	-27.330	16.898
-10	4	5	82.624		82.549	-82.180	7.794
-10	4	4	60.280		42.242	42.060	3.917
-10	4	3	70.162		63.573	-47.562	-42.183
-10	4	2	65.504		74.172	-73.503	-9.941
-10	4	1	83.394		71.861	-65.875	28.714
-10	2	18	65.923		63.893	62.799	11.773
-10	2	17	61.860		58.889	-58.765	3.813
-10	2	16	39.451		43.257	39.810	-16.923
-10	2	15	0.0	*	23.402	-19.247	13.312
-10	2	14	63.173		64.790	64.118	-9.313

JCAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-10	2	13	70.147		75.479	-75.138	7.159
-10	2	12	87.535		79.273	-78.616	-10.183
-10	2	11	15.742	*	18.798	-3.834	18.403
-10	2	10	69.654		63.540	-63.305	-5.464
-10	2	9	19.058		20.964	20.493	4.418
-10	2	8	84.110		83.928	-81.554	-19.822
-10	2	7	94.032		89.858	85.055	28.985
-10	2	6	100.141		111.511	-107.465	-29.767
-10	2	5	19.182		23.713	-22.787	6.562
-10	2	4	109.020		131.469	-130.992	-11.185
-10	2	3	57.188		67.933	-66.856	12.050
-10	2	2	62.880		67.754	-66.604	12.428
-10	2	1	34.213		40.645	-40.237	-5.740
-10	0	18	22.365		21.870	-20.645	-7.218
-10	0	17	24.820		35.046	34.473	6.309
-10	0	16	67.990		74.423	-73.683	-10.469
-10	0	15	4.568	*	15.765	15.446	3.156
-10	0	14	30.163		40.546	-40.091	-6.056
-10	0	13	29.579		12.478	-12.477	-0.119
-10	0	12	51.450		37.287	37.252	1.628
-10	0	11	17.687		13.173	12.159	-5.069
-10	0	10	43.235		33.960	33.621	4.782
-10	0	9	176.184		168.690	-168.030	-14.910
-10	0	8	86.218		84.677	84.433	6.421
-10	0	7	152.758		153.635	-152.657	-17.307
-10	0	6	20.013		29.891	29.180	6.480
-10	0	5	142.776		148.827	-148.143	-14.251
-10	0	4	148.609		154.626	154.491	6.467
-10	0	3	49.235		61.622	-60.969	-8.941
-10	0	2	70.781		67.640	-67.546	-3.578
-10	0	1	78.408		82.609	-82.367	-6.325
-9	1	18	35.255		40.019	24.437	31.692
-9	1	17	72.347		82.069	75.821	-31.408
-9	1	16	76.290		78.728	54.607	56.711
-9	1	15	67.460		62.605	51.716	35.282
-9	1	14	79.130		64.755	52.710	-37.614
-9	1	13	76.840		80.961	69.939	40.784
-9	1	12	113.444		105.958	90.402	-55.270
-9	1	11	94.436		94.037	64.906	68.046
-9	1	10	121.480		115.101	64.372	-95.418
-9	1	9	90.615		85.600	76.009	39.370
-9	1	8	100.174		106.958	105.080	19.954
-9	1	7	128.253		123.291	71.473	100.460
-9	1	6	64.000		70.038	52.722	-46.105
-9	1	5	126.901		125.801	109.991	-61.057
-9	1	4	102.748		127.943	109.960	65.408
-9	1	3	68.699		75.649	58.333	-48.166
-9	1	2	54.630		72.405	25.344	67.824
-9	1	1	180.890		196.285	127.719	-149.050
-9	3	18	62.681		60.309	59.723	8.388
-9	3	17	44.512		53.734	42.763	32.537
-9	3	16	65.594		69.000	43.005	-53.958
-9	3	15	88.383		75.245	57.432	-46.616

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
-9	3	14	103.342	103.823	65.975	80.166
-9	3	13	77.286	68.560	54.909	-41.055
-9	3	12	75.779	75.437	50.098	56.399
-9	3	11	105.514	99.854	73.969	-67.078
-9	3	10	165.981	164.782	97.877	132.563
-9	3	9	103.397	101.145	39.524	-93.103
-9	3	8	104.078	97.380	98.717	40.150
-9	3	7	121.728	114.762	66.335	-93.648
-9	3	6	101.614	109.869	90.807	61.850
-9	3	5	40.506	36.057	30.987	-18.436
-9	3	4	97.423	95.163	95.055	4.522
-9	3	3	87.931	97.735	64.882	73.092
-9	3	2	108.131	114.223	93.264	-65.944
-9	3	1	103.317	107.753	56.279	91.889
-9	5	17	43.759	35.878	35.574	4.658
-9	5	16	47.991	56.534	50.107	26.181
-9	5	15	69.169	67.860	40.812	54.215
-9	5	14	103.267	101.810	100.731	-14.784
-9	5	13	60.765	58.759	48.114	33.730
-9	5	12	95.504	88.107	50.772	-72.008
-9	5	11	119.779	113.940	60.119	96.789
-9	5	10	119.819	110.817	88.352	-66.891
-9	5	9	61.114	64.589	48.752	42.367
-9	5	8	85.135	76.456	75.645	-11.102
-9	5	7	165.414	161.418	84.945	137.259
-9	5	6	112.085	107.594	100.923	-37.295
-9	5	5	61.199	65.624	52.102	-39.899
-9	5	4	85.806	84.629	69.943	47.644
-9	5	3	72.880	84.539	84.259	-6.878
-9	5	2	65.751	67.161	61.761	26.385
-9	5	1	97.099	94.999	47.923	-82.025
-9	7	16	57.844	52.065	15.859	-49.591
-9	7	15	60.652	67.770	67.243	-8.435
-9	7	14	75.170	68.451	39.823	55.674
-9	7	13	54.967	56.013	53.544	-16.448
-9	7	12	65.298	56.240	39.831	39.704
-9	7	11	89.801	89.395	89.127	-6.927
-9	7	10	145.514	132.705	73.539	110.466
-9	7	9	91.635	83.144	59.348	-58.229
-9	7	8	36.921	34.323	34.322	0.210
-9	7	7	89.642	85.911	84.006	-17.994
-9	7	6	79.514	69.643	53.329	44.790
-9	7	5	52.050	60.411	49.669	34.387
-9	7	4	75.887	63.656	63.339	6.347
-9	7	3	108.107	113.282	92.802	64.966
-9	7	2	73.461	77.455	63.072	-44.958
-9	7	1	106.518	109.687	48.819	98.223
-9	9	14	46.581	45.142	45.000	-3.582
-9	9	13	66.982	54.944	52.084	17.496
-9	9	12	54.305	62.226	47.963	-39.643
-9	9	11	53.985	50.607	36.411	35.148
-9	9	10	55.046	46.774	23.601	-40.383
-9	9	9	84.182	73.886	66.721	31.741

JCAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-9	9	8	62.190		55.714	51.132	22.127
-9	9	7	97.070		89.500	77.257	45.184
-9	9	6	46.305		36.666	36.515	-3.321
-9	9	5	79.975		81.924	74.321	-34.467
-9	9	4	43.740		47.748	37.789	29.188
-9	9	3	46.561		50.607	39.820	-31.233
-9	9	2	31.370		40.221	22.149	33.573
-9	9	1	60.817		57.508	41.401	-39.913
-9	11	11	63.976		55.773	49.274	-26.128
-9	11	10	75.451		70.554	54.851	44.376
-9	11	9	52.505		40.212	32.177	-24.116
-9	11	8	53.732		44.828	37.472	24.606
-9	11	7	61.316		41.585	9.196	-40.556
-9	11	6	69.085		62.820	61.046	14.823
-9	11	5	17.890	*	37.106	22.399	29.583
-9	11	4	59.790		51.657	47.173	21.051
-9	11	3	71.179		59.002	55.278	20.630
-9	11	2	67.910		67.610	66.280	-13.346
-9	11	1	43.389		48.219	20.749	43.527
-9	13	6	57.068		42.876	39.797	-15.956
-9	13	5	49.832		50.415	47.231	17.632
-9	13	4	0.0	*	14.293	13.938	3.169
-9	13	3	18.169	*	20.237	9.896	-17.652
-9	13	2	56.155		50.598	44.443	24.187
-9	13	1	29.650		26.546	25.303	8.026
-8	12	10	52.480		36.504	31.149	19.035
-8	12	9	32.468		42.265	41.353	-8.729
-8	12	8	25.500		25.765	1.403	-25.727
-8	12	7	49.957		45.148	23.972	38.258
-8	12	6	43.548		46.810	-8.691	45.996
-8	12	5	94.472		90.954	88.758	-19.865
-8	12	4	27.926		29.666	0.996	-29.649
-8	12	3	66.193		65.744	65.740	0.758
-8	12	2	30.275		32.050	22.243	23.075
-8	12	1	94.918		78.502	75.772	-20.524
-8	10	14	29.479		25.891	-15.844	-20.477
-8	10	13	57.224		53.977	53.315	8.425
-8	10	12	9.326	*	3.398	2.387	-2.419
-8	10	11	58.135		44.057	43.382	7.685
-8	10	10	45.482		27.526	-26.358	7.936
-8	10	9	62.609		51.300	51.208	-3.060
-8	10	8	54.698		67.436	64.553	-19.508
-8	10	7	44.212		37.297	36.771	-6.239
-8	10	6	68.687		81.257	76.270	-27.756
-8	10	5	9.573	*	5.273	4.445	2.838
-8	10	4	87.354		89.619	88.286	15.404
-8	10	3	47.015		43.590	-14.452	41.124
-8	10	2	105.853		93.418	85.208	-38.296
-8	10	1	12.883	*	26.803	26.514	-3.922
-8	8	16	69.963		64.237	62.907	-13.007
-8	8	15	48.796		41.402	-41.361	1.836
-8	8	14	55.402		48.417	41.197	25.436
-8	8	13	29.286		26.265	-17.448	-10.191

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-8	8	12	128.340		121.214	112.910	-44.093
-8	8	11	9.230	*	4.888	3.801	-3.073
-8	8	10	60.087		51.586	51.225	6.092
-8	8	9	15.482	*	22.404	22.249	-2.628
-8	8	8	97.639		86.619	77.164	-39.352
-8	8	7	47.145		51.466	39.334	33.190
-8	8	6	33.625		34.530	-26.181	22.514
-8	8	5	109.323		114.627	111.637	-26.008
-8	8	4	32.602		44.344	30.543	-32.148
-8	8	3	129.383		124.235	124.215	-2.209
-8	8	2	15.835	*	34.877	34.837	1.663
-8	8	1	106.430		96.230	95.884	8.148
-8	6	17	37.214		35.046	34.703	4.894
-8	6	16	20.099		12.027	-7.917	9.054
-8	6	15	97.753		100.099	96.366	-27.083
-8	6	14	28.377		31.110	-28.719	-11.960
-8	6	13	82.396		72.809	72.138	9.859
-8	6	12	50.355		45.642	-23.245	39.280
-8	6	11	70.771		67.687	61.507	-28.255
-8	6	10	21.319		18.929	-9.423	16.417
-8	6	9	78.178		70.730	58.683	-39.485
-8	6	8	88.241		99.432	74.177	66.215
-8	6	7	45.860		38.103	28.953	-24.770
-8	6	6	109.645		122.707	120.912	-20.910
-8	6	5	5.773	*	7.369	-0.652	-7.341
-8	6	4	141.709		146.941	137.082	52.919
-8	6	3	55.032		54.033	-53.234	9.258
-8	6	2	118.487		114.862	113.974	-14.252
-8	6	1	27.457		42.746	42.742	-0.561
-8	4	18	27.238		23.488	23.436	1.562
-8	4	17	0.0	*	8.316	-6.829	-4.745
-8	4	16	41.273		36.183	35.213	8.324
-8	4	15	59.018		56.452	-56.207	-5.255
-8	4	14	85.489		85.179	82.951	19.354
-8	4	13	31.038		33.930	-29.498	-16.767
-8	4	12	66.053		64.946	64.854	-3.449
-8	4	11	14.171	*	13.138	12.490	-4.077
-8	4	10	104.776		99.240	98.231	14.109
-8	4	9	49.960		55.853	55.748	-3.431
-8	4	8	29.054		33.802	-33.310	-5.746
-8	4	7	65.188		67.702	66.972	9.914
-8	4	6	26.726		26.489	-17.527	19.862
-8	4	5	178.371		195.700	194.908	-17.583
-8	4	4	44.486		39.719	-39.555	3.604
-8	4	3	166.796		163.344	163.280	4.578
-8	4	2	42.160		36.107	-35.097	-8.480
-8	4	1	192.905		188.301	187.224	20.111
-8	2	18	33.873		33.672	-15.076	-30.109
-8	2	17	79.188		70.075	66.128	23.189
-8	2	16	36.182		28.309	-28.244	-1.923
-8	2	15	99.020		90.636	90.019	10.564
-8	2	14	25.255		26.880	-15.467	-21.985
-8	2	13	97.455		100.613	99.173	16.960

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F (OBS)		F (CALC)	A (CALC)	B (CALC)
-8	2	12	55.641		61.191	-61.061	-3.984
-8	2	11	65.283		71.369	69.858	14.608
-8	2	10	46.259		38.824	38.712	-2.954
-8	2	9	26.072		31.299	29.627	10.093
-8	2	8	77.673		70.374	70.223	-4.605
-8	2	7	66.152		70.302	69.812	8.286
-8	2	6	164.213		167.299	166.925	-11.193
-8	2	5	83.973		87.217	-84.029	23.365
-8	2	4	160.628		175.351	172.839	29.571
-8	2	3	17.915		8.331	-8.319	0.444
-8	2	2	159.669		165.210	163.213	-25.606
-8	2	1	49.001		36.776	-35.591	9.259
-8	0	18	81.294		65.041	64.589	7.656
-8	0	17	0.930	*	4.130	0.752	-4.061
-8	0	16	72.116		61.569	60.760	9.951
-8	0	15	105.486		101.821	-101.241	-10.845
-8	0	14	138.246		139.363	138.682	13.753
-8	0	13	17.560	*	27.900	-26.646	-8.270
-8	0	12	117.214		127.782	126.883	15.135
-8	0	11	16.546		18.267	-18.097	-2.484
-8	0	10	147.581		155.944	155.413	12.854
-8	0	9	15.829		16.060	-15.944	1.927
-8	0	8	65.979		75.378	75.327	2.763
-8	0	7	125.511		120.210	119.977	7.482
-8	0	6	35.005		37.530	37.494	-1.646
-8	0	5	84.299		85.321	84.099	14.389
-8	0	4	19.760	*	15.355	15.288	-1.431
-8	0	3	296.658		310.146	309.543	19.337
-8	0	2	20.246		15.093	15.091	-0.254
-8	0	1	85.523		89.350	88.296	13.685
-7	1	19	36.037		35.820	-34.884	-8.138
-7	1	18	92.352		101.980	-65.374	-78.269
-7	1	17	99.875		97.650	-67.476	70.587
-7	1	16	49.756		63.644	-34.422	-53.532
-7	1	15	50.705		55.099	-53.930	11.289
-7	1	14	75.551		75.684	-72.680	-21.113
-7	1	13	94.914		102.622	-79.046	65.444
-7	1	12	75.825		75.303	-74.778	-8.873
-7	1	11	136.157		138.927	-54.779	-127.672
-7	1	10	104.783		101.715	-98.432	25.632
-7	1	9	105.176		111.646	-65.844	-90.163
-7	1	8	186.409		178.854	-98.819	149.076
-7	1	7	149.884		154.013	-47.385	-146.542
-7	1	6	162.362		176.471	-119.586	129.773
-7	1	5	104.187		112.517	-92.626	-63.880
-7	1	4	69.707		77.024	-64.823	41.601
-7	1	3	115.040		131.586	-40.248	-125.279
-7	1	2	122.411		145.333	-142.958	-26.166
-7	1	1	81.569		77.999	-77.959	2.507
-7	3	18	83.909		81.760	-47.644	66.443
-7	3	17	80.489		84.591	-45.238	-71.478
-7	3	16	68.356		71.102	-51.774	48.734
-7	3	15	116.128		129.710	-93.528	-89.873

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
-7	3	14	62.833	62.024	-60.270	14.648
-7	3	13	87.926	94.936	-61.550	-72.281
-7	3	12	46.856	47.383	-46.499	9.114
-7	3	11	117.129	117.273	-112.609	32.745
-7	3	10	37.126	36.966	-36.950	-1.060
-7	3	9	113.922	110.157	-109.510	11.924
-7	3	8	160.804	170.021	-76.325	-151.926
-7	3	7	156.278	159.189	-108.402	116.576
-7	3	6	116.493	129.274	-74.572	-105.598
-7	3	5	81.083	94.026	-86.062	-37.871
-7	3	4	127.267	135.674	-84.597	-106.070
-7	3	3	140.001	142.875	-80.735	117.877
-7	3	2	85.410	90.983	-47.844	77.388
-7	3	1	155.978	166.303	-112.321	-125.339
-7	5	18	93.008	93.823	-36.729	-86.335
-7	5	17	83.666	85.450	-36.591	77.219
-7	5	16	67.626	71.268	-45.809	-54.596
-7	5	15	71.769	68.483	-66.932	14.494
-7	5	14	27.806	36.965	-36.199	-7.485
-7	5	13	89.505	85.946	-39.595	76.282
-7	5	12	83.609	90.220	-77.641	-45.952
-7	5	11	131.953	130.316	-97.187	-86.816
-7	5	10	55.745	63.573	-55.264	31.423
-7	5	9	62.054	59.932	-54.772	-24.330
-7	5	8	81.560	83.904	-73.533	40.408
-7	5	7	117.373	114.423	-62.659	-95.742
-7	5	6	131.110	128.163	-15.260	127.251
-7	5	5	110.163	101.120	-94.970	-34.728
-7	5	4	92.416	100.386	-98.707	18.285
-7	5	3	110.493	97.819	-82.630	-52.353
-7	5	2	47.726	72.168	-27.695	-66.642
-7	5	1	76.378	63.706	-61.192	17.719
-7	7	16	75.676	69.666	-58.655	37.588
-7	7	15	77.043	79.346	-63.043	-48.181
-7	7	14	55.422	54.096	-53.073	10.468
-7	7	13	51.428	57.830	-47.666	-32.747
-7	7	12	73.133	69.736	-61.548	-32.787
-7	7	11	56.678	59.567	-40.017	44.123
-7	7	10	45.744	37.143	-33.795	15.411
-7	7	9	65.283	75.886	-52.200	55.080
-7	7	8	162.596	168.643	-106.795	-130.519
-7	7	7	100.237	105.459	-65.942	82.299
-7	7	6	96.174	97.113	-64.118	-72.937
-7	7	5	59.901	51.631	-45.802	23.830
-7	7	4	120.334	109.843	-74.359	-80.847
-7	7	3	120.912	101.349	-18.607	99.626
-7	7	2	50.134	52.416	-43.584	29.119
-7	7	1	66.843	76.655	-58.452	-49.592
-7	9	15	29.610	9.025	-8.610	2.707
-7	9	14	52.386	44.203	-43.606	-7.238
-7	9	13	54.203	43.464	-37.813	21.430
-7	9	12	78.505	85.673	-85.647	-2.110
-7	9	11	87.252	85.711	-40.593	-75.489

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-7	9	10	71.397		78.283	-77.311	12.298
-7	9	9	75.664		74.245	-46.768	-57.664
-7	9	8	70.240		63.831	-47.609	42.518
-7	9	7	91.110		85.034	-38.246	-75.947
-7	9	6	92.057		80.297	-37.823	70.831
-7	9	5	89.878		76.602	-61.221	-46.041
-7	9	4	79.669		69.615	-64.207	26.901
-7	9	3	110.199		89.369	-60.481	-65.794
-7	9	2	65.517		75.174	-65.655	-36.614
-7	9	1	69.745		53.391	-51.070	-15.570
-7	11	13	72.484		77.039	-66.668	-38.605
-7	11	12	34.371		11.887	-9.982	6.455
-7	11	11	44.882		46.556	-44.300	14.317
-7	11	10	42.873		34.360	-24.103	-24.487
-7	11	9	53.191		57.316	-57.117	4.769
-7	11	8	54.742		50.775	-41.860	-28.738
-7	11	7	78.440		78.516	-72.032	31.244
-7	11	6	103.216		97.357	-65.148	-72.347
-7	11	5	42.709		48.172	-47.021	-10.470
-7	11	4	45.653		36.347	-22.000	-28.933
-7	11	3	58.366		47.482	-43.232	19.634
-7	11	2	31.382		20.610	-15.224	13.892
-7	11	1	35.792		46.618	-42.698	-18.713
-7	13	9	49.389		51.444	-43.003	-28.235
-7	13	8	28.599		21.178	0.008	21.178
-7	13	7	51.482		42.720	-34.634	-25.009
-7	13	6	31.838		23.770	-22.205	8.482
-7	13	5	43.177		27.596	-25.587	-10.336
-7	13	4	53.959		39.580	-33.208	21.535
-7	13	3	88.456		79.446	-74.488	-27.626
-7	13	2	35.551		60.798	-36.694	-48.477
-7	13	1	16.296	*	20.406	-17.674	10.199
-6	14	7	64.577		49.865	-40.207	-29.495
-6	14	6	15.884	*	26.306	-25.765	5.304
-6	14	5	36.742		29.220	-29.132	-2.258
-6	14	4	29.557		36.816	-36.651	-3.478
-6	14	3	50.144		41.033	-40.295	-7.748
-6	14	2	70.627		75.721	-65.733	37.589
-6	14	1	25.675		31.334	-29.477	10.625
-6	12	11	39.520		29.680	17.826	-23.731
-6	12	10	82.567		69.234	-68.947	-6.301
-6	12	9	17.759	*	14.423	5.673	-13.260
-6	12	8	67.666		57.704	-54.856	17.904
-6	12	7	19.834		41.095	-38.353	14.761
-6	12	6	105.389		92.372	-86.850	31.460
-6	12	5	29.885		49.840	-49.766	-2.699
-6	12	4	51.753		39.720	-38.616	-9.303
-6	12	3	50.134		61.078	-61.078	-0.042
-6	12	2	45.956		38.984	-38.912	2.381
-6	12	1	51.246		62.600	-46.640	-41.756
-6	10	14	12.341	*	5.967	5.430	-2.473
-6	10	13	57.798		60.782	-55.940	23.773
-6	10	12	37.096		29.121	7.246	-28.206

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-6	10	11	65.500		68.663	-68.298	-7.071
-6	10	10	24.721		31.148	-18.385	25.144
-6	10	9	140.559		136.324	-116.493	70.806
-6	10	8	68.705		60.937	-4.453	-60.774
-6	10	7	69.782		60.515	-40.513	-44.954
-6	10	6	25.196		36.248	-36.235	0.973
-6	10	5	57.171		53.091	-42.094	32.353
-6	10	4	69.442		76.534	-56.266	-51.880
-6	10	3	56.386		47.042	-45.861	10.471
-6	10	2	128.162		145.154	-142.242	28.930
-6	10	1	33.564		37.316	-11.942	35.354
-6	8	16	26.218		15.414	-10.447	11.334
-6	8	15	42.181		44.864	-32.490	30.938
-6	8	14	61.282		61.362	-57.466	-21.517
-6	8	13	44.879		39.386	-37.848	10.896
-6	8	12	75.085		70.150	-69.827	6.721
-6	8	11	46.066		38.364	37.039	-9.996
-6	8	10	91.810		84.088	-76.397	-35.132
-6	8	9	32.752		29.365	-4.010	-29.090
-6	8	8	76.247		64.848	-64.839	1.077
-6	8	7	52.714		61.033	-50.172	34.753
-6	8	6	130.074		114.020	-112.958	15.523
-6	8	5	88.583		108.458	-104.236	-29.970
-6	8	4	29.014		21.868	-13.515	-17.191
-6	8	3	85.823		102.435	-102.435	0.243
-6	8	2	34.069		36.263	5.033	-35.912
-6	8	1	131.609		136.983	-124.945	-56.152
-6	6	17	37.017		37.787	-36.629	-9.284
-6	6	16	46.371		49.001	-41.899	25.407
-6	6	15	23.096		38.910	-1.649	-38.875
-6	6	14	17.553	*	21.175	16.736	12.973
-6	6	13	78.266		84.607	-81.050	-24.272
-6	6	12	26.487		30.459	21.646	21.429
-6	6	11	134.291		129.854	-129.646	-7.349
-6	6	10	45.661		43.077	-13.413	40.935
-6	6	9	174.864		177.399	-177.225	7.863
-6	6	8	12.971	*	12.815	-2.692	-12.530
-6	6	7	74.882		66.769	-59.307	-30.671
-6	6	6	0.0	*	36.647	-36.283	5.152
-6	6	5	73.893		58.898	-57.688	-11.881
-6	6	4	91.298		103.890	-103.846	3.010
-6	6	3	78.982		68.827	-68.553	6.133
-6	6	2	204.771		224.584	-216.859	58.398
-6	6	1	59.748		56.712	-39.013	-41.161
-6	4	18	24.441		26.555	17.512	-19.962
-6	4	17	25.960		27.504	-22.588	-15.692
-6	4	16	19.263		18.955	-15.018	11.565
-6	4	15	49.442		53.666	-47.425	25.117
-6	4	14	128.515		127.344	-126.420	-15.312
-6	4	13	22.275		3.831	3.820	-0.287
-6	4	12	143.183		139.122	-137.803	19.106
-6	4	11	63.812		57.216	55.516	-13.844
-6	4	10	158.443		152.723	-149.628	-30.591

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-6	4	9	92.633		91.742	90.119	-17.181
-6	4	8	175.601		168.365	-167.907	12.411
-6	4	7	84.567		92.767	-87.881	29.710
-6	4	6	191.714		189.671	-189.636	3.614
-6	4	5	114.709		129.639	-122.372	-42.794
-6	4	4	85.114		74.924	-68.536	30.273
-6	4	3	94.908		106.805	-103.537	-26.216
-6	4	2	34.078		32.261	-27.132	-17.453
-6	4	1	159.241		163.738	-149.528	-66.719
-6	2	18	82.269		97.479	-97.266	-6.439
-6	2	17	38.683		24.965	-24.636	4.038
-6	2	16	13.909	*	26.142	-25.989	-2.824
-6	2	15	58.818		45.375	-43.674	-12.308
-6	2	14	33.229		27.239	26.730	-5.241
-6	2	13	63.394		53.550	-51.316	15.309
-6	2	12	26.696		26.691	17.477	-20.173
-6	2	11	218.182		215.054	-215.024	-3.605
-6	2	10	22.855		16.712	16.578	-2.113
-6	2	9	195.670		198.463	-195.146	36.132
-6	2	8	36.776		34.891	-31.885	-14.169
-6	2	7	122.343		121.853	-114.265	-42.328
-6	2	6	51.192		46.759	45.267	-11.715
-6	2	5	70.768		63.658	-53.777	34.063
-6	2	4	214.191		227.061	-225.476	-26.776
-6	2	3	94.455		96.928	-95.000	19.233
-6	2	2	188.798		206.141	-205.062	-21.063
-6	2	1	119.320		118.963	-114.041	33.864
-6	0	19	59.360		71.633	-70.768	-11.094
-6	0	18	25.149		46.528	46.021	6.854
-6	0	17	14.474	*	10.313	-7.505	-7.073
-6	0	16	0.0	*	19.963	19.958	-0.459
-6	0	15	76.655		94.589	-94.407	-5.865
-6	0	14	107.207		96.540	-95.978	-10.406
-6	0	13	13.401	*	7.175	7.146	0.650
-6	0	12	91.634		89.539	-88.528	-13.416
-6	0	11	15.386	*	5.087	1.534	4.850
-6	0	10	63.787		67.406	-66.033	-13.536
-6	0	9	99.841		110.354	110.263	4.481
-6	0	8	178.199		187.251	-186.667	-14.785
-6	0	7	124.756		108.405	-108.281	-5.191
-6	0	6	69.313		79.387	-78.698	-10.437
-6	0	5	186.730		178.288	-177.906	-11.671
-6	0	4	33.413		38.809	-38.749	-2.151
-6	0	3	152.662		149.237	-148.378	-15.985
-6	0	2	203.414		205.407	205.324	5.827
-6	0	1	273.435		283.204	-282.359	-21.851
-5	1	19	58.021		63.467	63.335	4.091
-5	1	18	52.955		49.729	48.775	9.697
-5	1	17	99.179		92.347	50.704	-77.182
-5	1	16	53.191		56.089	38.861	40.445
-5	1	15	111.469		107.822	88.099	-62.162
-5	1	14	164.469		167.814	32.308	164.674
-5	1	13	100.890		106.960	86.222	-63.294

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
-5	1	12	98.347	106.975	14.391	85.425
-5	1	11	124.149	135.594	93.877	-97.840
-5	1	10	57.566	53.041	45.327	27.546
-5	1	9	82.191	91.434	81.346	-41.748
-5	1	8	112.502	102.244	82.562	-60.310
-5	1	7	107.068	103.857	91.467	49.194
-5	1	6	101.366	105.350	90.930	53.201
-5	1	5	195.139	186.371	63.039	175.386
-5	1	4	152.125	152.311	90.107	-122.798
-5	1	3	104.383	102.502	88.544	51.640
-5	1	2	171.372	187.258	75.825	-171.220
-5	1	1	56.998	48.611	42.376	23.819
-5	3	18	55.073	55.511	55.184	-6.019
-5	3	17	71.994	74.252	22.561	70.742
-5	3	16	84.025	87.941	87.141	11.835
-5	3	15	49.692	52.240	45.157	26.266
-5	3	14	161.607	160.314	59.549	-148.844
-5	3	13	72.459	80.098	29.960	74.284
-5	3	12	81.126	81.676	78.063	-24.025
-5	3	11	61.628	63.555	60.192	20.401
-5	3	10	75.636	77.450	73.174	-25.379
-5	3	9	129.647	126.288	81.307	96.632
-5	3	8	126.543	130.797	88.060	96.712
-5	3	7	161.455	162.299	41.287	-156.959
-5	3	6	83.566	85.768	77.495	-36.753
-5	3	5	148.371	153.117	35.197	-149.017
-5	3	4	215.567	224.401	73.560	212.001
-5	3	3	160.534	163.109	47.034	-156.180
-5	3	2	216.795	220.834	128.258	179.771
-5	3	1	126.419	122.035	-3.217	-121.993
-5	5	18	27.010	22.497	22.105	-4.185
-5	5	17	73.157	69.286	46.497	-51.367
-5	5	16	75.173	67.909	53.700	41.569
-5	5	15	61.644	54.495	49.677	-22.402
-5	5	14	120.169	118.764	61.780	101.430
-5	5	13	75.229	74.482	73.943	-8.938
-5	5	12	115.479	116.086	96.706	64.217
-5	5	11	69.716	65.353	19.239	-62.458
-5	5	10	78.074	76.661	74.982	15.957
-5	5	9	81.960	79.663	78.556	13.234
-5	5	8	95.123	97.263	59.614	-76.852
-5	5	7	69.208	74.162	30.720	67.501
-5	5	6	149.052	146.494	124.716	76.853
-5	5	5	191.912	205.683	108.289	174.869
-5	5	4	212.542	216.509	100.218	-191.918
-5	5	3	83.270	76.315	-2.037	76.288
-5	5	2	98.884	101.642	88.492	-50.003
-5	5	1	101.881	95.232	45.865	83.459
-5	7	17	85.997	81.416	53.219	61.615
-5	7	16	62.452	61.975	61.878	3.477
-5	7	15	66.985	65.316	46.018	46.352
-5	7	14	117.800	114.621	23.659	-112.153
-5	7	13	102.948	100.931	62.030	79.620

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
-5	7	12	50.915	38.618	26.531	-28.061
-5	7	11	103.397	103.385	77.776	68.113
-5	7	10	65.007	61.969	60.719	-12.381
-5	7	9	124.188	122.627	95.283	77.191
-5	7	8	64.820	68.182	51.642	44.518
-5	7	7	72.051	85.802	59.944	-61.390
-5	7	6	57.404	56.800	40.324	40.003
-5	7	5	79.071	85.921	65.205	-55.953
-5	7	4	51.932	55.094	-7.706	54.552
-5	7	3	91.681	95.712	91.449	-28.246
-5	7	2	204.001	193.038	87.508	172.064
-5	7	1	85.395	86.975	82.014	-28.955
-5	9	15	43.909	38.146	33.403	-18.422
-5	9	14	105.946	102.232	57.946	84.223
-5	9	13	87.626	85.803	76.791	-38.280
-5	9	12	80.091	80.286	52.681	60.586
-5	9	11	74.817	59.858	18.990	-56.766
-5	9	10	48.464	40.803	36.649	17.937
-5	9	9	54.018	41.956	40.713	-10.138
-5	9	8	39.236	44.176	38.559	-21.557
-5	9	7	59.350	58.067	44.221	37.634
-5	9	6	77.274	72.677	67.869	25.994
-5	9	5	109.199	109.131	88.445	63.930
-5	9	4	57.866	63.515	33.366	-54.045
-5	9	3	38.032	31.690	30.245	9.461
-5	9	2	38.336	33.455	-1.413	-33.425
-5	9	1	79.198	67.636	65.103	18.338
-5	11	13	29.697	21.740	6.411	20.773
-5	11	12	40.015	33.485	31.704	-10.774
-5	11	11	70.291	66.072	50.353	42.780
-5	11	10	61.280	57.180	57.096	3.090
-5	11	9	48.715	36.922	33.235	16.082
-5	11	8	66.687	67.057	51.665	42.748
-5	11	7	60.584	58.025	46.214	-35.088
-5	11	6	10.266 *	6.934	5.747	-3.879
-5	11	5	45.073	49.201	-8.670	-48.431
-5	11	4	113.762	105.261	56.966	88.514
-5	11	3	57.654	42.510	39.790	-14.963
-5	11	2	73.812	65.922	55.176	36.074
-5	11	1	59.008	46.767	18.054	-43.142
-5	13	10	34.484	33.478	33.466	0.916
-5	13	9	22.755	9.547	4.247	-8.550
-5	13	8	41.071	37.978	37.971	-0.760
-5	13	7	57.996	65.806	34.713	55.906
-5	13	6	45.901	49.298	48.483	-8.927
-5	13	5	60.717	57.757	43.826	37.619
-5	13	4	54.887	55.856	49.214	-26.418
-5	13	3	57.561	49.717	15.751	47.156
-5	13	2	58.546	58.628	-17.036	-56.099
-5	13	1	61.609	40.843	25.767	31.690
-4	14	8	21.058	18.049	15.772	8.776
-4	14	7	86.302	76.745	76.536	-5.658
-4	14	6	31.853	42.149	41.436	7.720

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CAIC)	A(CAIC)	B(CAIC)
-4	14	5	74.990	72.747	66.011	-30.573
-4	14	4	28.352	27.516	27.277	3.617
-4	14	3	60.411	38.577	38.471	-2.858
-4	14	2	63.046	62.991	35.399	52.103
-4	14	1	53.351	42.804	40.742	13.126
-4	12	12	38.786	50.478	15.378	48.078
-4	12	11	59.803	57.600	50.631	-27.463
-4	12	10	75.539	86.506	81.871	-27.936
-4	12	9	40.059	28.825	24.128	15.770
-4	12	8	50.812	54.779	49.979	22.425
-4	12	7	36.190	39.726	25.862	-30.154
-4	12	6	73.772	65.171	64.666	8.101
-4	12	5	78.141	71.561	12.544	70.453
-4	12	4	73.925	61.903	56.949	24.265
-4	12	3	58.973	82.874	78.492	-26.591
-4	12	2	81.776	64.151	62.914	-12.538
-4	12	1	85.784	96.875	94.541	21.135
-4	10	14	96.038	91.856	75.930	-51.693
-4	10	13	48.902	56.798	56.454	-6.250
-4	10	12	49.401	39.784	39.206	-6.753
-4	10	11	48.403	55.156	49.495	24.340
-4	10	10	30.533	20.960	5.451	-20.238
-4	10	9	63.108	72.994	68.591	24.969
-4	10	8	29.898	20.056	18.375	8.039
-4	10	7	155.932	157.299	156.645	14.319
-4	10	6	0.0 *	16.261	10.926	-12.043
-4	10	5	135.944	124.966	124.933	-2.843
-4	10	4	50.306	70.958	58.934	-39.521
-4	10	3	132.597	113.578	113.557	2.194
-4	10	2	51.170	40.868	15.333	37.882
-4	10	1	64.051	55.090	26.740	48.165
-4	8	16	26.986	16.976	-14.832	-8.259
-4	8	15	54.836	51.707	51.213	-7.129
-4	8	14	40.303	42.607	42.597	0.936
-4	8	13	29.264	27.294	23.744	13.459
-4	8	12	27.564	37.216	28.742	23.641
-4	8	11	48.272	47.027	42.060	-21.035
-4	8	10	153.191	159.928	159.284	-14.345
-4	8	9	44.761	36.299	36.055	4.206
-4	8	8	121.064	128.187	128.187	-0.097
-4	8	7	38.902	40.363	-11.357	-38.732
-4	8	6	148.645	145.646	145.476	-7.040
-4	8	5	77.226	75.962	-35.356	67.233
-4	8	4	179.358	166.615	166.529	5.352
-4	8	3	73.444	102.018	99.315	-20.609
-4	8	2	146.898	131.986	131.589	-10.228
-4	8	1	85.740	108.152	108.139	-1.710
-4	6	17	62.836	59.316	-50.909	-30.291
-4	6	16	87.704	85.209	85.191	1.792
-4	6	15	33.611	33.398	8.352	32.337
-4	6	14	106.433	100.111	96.357	27.157
-4	6	13	54.949	59.759	43.154	-41.338
-4	6	12	74.066	71.552	68.970	-19.049

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-4	6	11	100.461		103.091	100.415	23.238
-4	6	10	34.031		31.461	-16.209	26.964
-4	6	9	78.099		77.775	77.653	4.348
-4	6	8	30.135		26.312	5.320	25.769
-4	6	7	231.478		233.553	233.267	-11.565
-4	6	6	70.466		75.053	24.382	70.982
-4	6	5	210.256		197.651	182.934	-74.841
-4	6	4	52.575		58.098	54.662	19.684
-4	6	3	179.747		161.268	161.137	-6.481
-4	6	2	103.921		102.233	47.442	90.559
-4	6	1	60.418		35.225	26.864	-22.785
-4	4	18	9.285	*	8.686	-5.004	7.100
-4	4	17	119.199		118.888	118.888	-0.326
-4	4	16	39.095		44.844	-44.571	-4.943
-4	4	15	117.657		118.316	118.296	2.176
-4	4	14	31.626		32.246	-32.242	-0.531
-4	4	13	50.290		46.420	46.118	5.281
-4	4	12	41.233		45.593	27.349	36.479
-4	4	11	73.878		68.684	68.069	-9.168
-4	4	10	163.148		165.367	165.323	3.824
-4	4	9	38.096		38.267	34.180	-17.207
-4	4	8	141.376		139.556	135.588	33.043
-4	4	7	29.444		30.553	-9.185	-29.139
-4	4	6	205.957		203.342	203.216	7.141
-4	4	5	19.324		14.615	6.033	13.312
-4	4	4	106.827		108.250	33.439	68.963
-4	4	3	56.313		74.401	65.827	-34.676
-4	4	2	243.679		221.526	220.340	22.891
-4	4	1	255.940		282.836	281.447	-28.001
-4	2	18	49.260		49.707	49.706	0.234
-4	2	17	65.463		70.559	-70.195	7.157
-4	2	16	128.207		132.693	132.509	6.987
-4	2	15	15.473	*	25.124	-2.915	24.955
-4	2	14	68.212		81.331	75.998	-28.966
-4	2	13	76.628		65.762	65.178	8.749
-4	2	12	117.277		128.081	127.481	12.377
-4	2	11	116.447		99.658	90.226	42.320
-4	2	10	92.340		84.028	-73.488	-40.745
-4	2	9	159.488		150.210	150.202	1.617
-4	2	8	60.715		67.439	58.638	33.310
-4	2	7	191.270		180.676	174.681	46.157
-4	2	6	25.644		24.049	20.145	-13.135
-4	2	5	303.772		303.854	303.661	10.844
-4	2	4	86.206		88.196	86.836	-15.427
-4	2	3	149.941		155.749	151.949	34.192
-4	2	2	79.809		93.510	91.617	-18.720
-4	2	1	41.714		49.141	33.234	36.199
-4	0	19	88.302		86.870	86.036	12.007
-4	0	18	22.665		9.298	8.786	-3.043
-4	0	17	109.510		115.113	114.027	15.771
-4	0	16	18.459		3.299	2.062	-2.576
-4	0	15	85.792		97.171	96.402	12.198
-4	0	14	16.762	*	1.785	1.539	-0.904

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CAIC)	B(CAIC)
-4	0	13	55.642		69.623	69.380	5.807
-4	0	12	122.829		105.081	104.798	7.714
-4	0	11	37.860		27.761	-27.708	1.706
-4	0	10	220.383		212.141	211.340	18.412
-4	0	9	127.180		127.449	127.447	-0.730
-4	0	8	306.730		299.199	298.324	22.867
-4	0	7	164.570		164.472	-164.310	-7.302
-4	0	6	286.934		288.532	287.739	21.379
-4	0	5	10.815	*	9.850	8.866	-4.291
-4	0	4	380.109		373.598	373.153	18.219
-4	0	3	61.866		63.240	-63.164	3.097
-4	0	2	393.452		397.143	396.808	16.322
-4	0	1	281.680		281.730	281.379	14.070
-3	1	18	21.731		41.446	-37.614	17.406
-3	1	17	65.581		88.288	-34.052	-81.457
-3	1	16	67.376		78.294	-77.689	9.712
-3	1	15	52.996		35.306	-29.596	19.250
-3	1	14	61.207		63.097	-49.963	-38.535
-3	1	13	95.070		90.114	-81.901	37.589
-3	1	12	71.717		73.354	-61.616	-39.803
-3	1	11	111.993		104.291	-44.111	94.503
-3	1	10	170.755		173.357	-40.108	-168.653
-3	1	9	110.639		115.986	-108.329	41.444
-3	1	8	87.717		87.282	-72.250	-48.971
-3	1	7	83.994		87.005	-38.247	78.148
-3	1	6	84.748		78.377	-64.693	-44.247
-3	1	5	125.455		125.159	-53.614	-113.094
-3	1	4	207.503		195.707	-112.615	160.060
-3	3	18	20.968	*	36.113	-31.405	-17.829
-3	3	17	57.380		59.219	-56.256	18.498
-3	3	16	50.109		50.992	-50.314	-8.286
-3	3	15	67.012		62.468	-50.122	-37.285
-3	3	14	54.312		54.264	-49.595	22.021
-3	3	13	112.668		119.105	-72.076	-94.820
-3	3	12	92.955		84.666	-50.310	68.097
-3	3	11	143.457		148.355	-63.577	-134.042
-3	3	10	132.359		128.144	-85.921	95.071
-3	3	9	114.062		114.578	-72.689	-88.568
-3	3	8	163.116		158.796	0.599	158.795
-3	3	7	220.502		221.510	-133.725	-176.590
-3	3	6	46.884		57.625	-54.078	-19.906
-3	3	5	125.188		117.669	-113.551	-30.858
-3	3	4	22.514		30.506	-0.114	-30.506
-3	3	3	102.094		100.320	-93.681	35.889
-3	3	2	162.581		169.828	-96.216	-139.943
-3	3	1	142.577		154.699	-44.311	148.217
-3	5	17	85.238		96.893	-79.683	-55.127
-3	5	16	39.332		36.928	-36.590	-4.980
-3	5	15	61.893		66.242	-44.429	49.133
-3	5	14	82.670		70.861	-25.689	-66.040
-3	5	13	80.144		81.680	-66.242	47.788
-3	5	12	41.623		37.070	-31.089	-20.190
-3	5	11	112.422		113.174	-66.272	91.741

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)	F(CALC)	A(CALC)	B(CALC)
-3	5	10	162.514	159.688	-43.087	-153.765
-3	5	9	81.092	81.426	-63.435	51.051
-3	5	8	67.878	66.891	-33.631	-57.822
-3	5	7	102.265	98.248	-70.189	68.748
-3	5	6	91.366	83.523	-55.279	-62.612
-3	5	5	87.405	77.423	-29.929	71.404
-3	5	4	42.091	59.303	-14.793	57.428
-3	5	3	134.487	151.337	-85.247	-125.043
-3	5	2	70.283	79.015	14.757	77.625
-3	5	1	79.960	75.750	-31.609	-68.840
-3	7	16	27.076	30.967	-29.429	-9.636
-3	7	15	38.132	28.731	-28.496	-3.672
-3	7	14	84.258	89.393	-89.387	-0.961
-3	7	13	68,640	73.445	-28.153	-67.835
-3	7	12	51.644	56.093	-35.334	43.565
-3	7	11	79.030	74.643	-45.503	-59.169
-3	7	10	108.755	108.604	-85.551	66.901
-3	7	9	27.999	25.057	-9.159	-23.323
-3	7	8	88.346	79.052	-17.878	77.004
-3	7	7	128.057	118.211	-62.938	-100.064
-3	7	6	85.835	84.968	-84.659	7.239
-3	7	5	47.598	66.792	-8.148	66.293
-3	7	4	74.209	87.584	-48.411	-72.989
-3	7	3	67.522	56.057	-55.621	-6.976
-3	7	2	63.812	88.035	-70.123	-53.226
-3	7	1	226.428	239.652	33.632	237.281
-3	9	15	35.077	40.010	-39.062	8.655
-3	9	14	43.807	36.354	-32.416	-16.455
-3	9	13	37.885	38.357	-34.793	16.146
-3	9	12	55.650	45.273	-37.467	-25.414
-3	9	11	50.577	49.628	-28.931	40.323
-3	9	10	96.312	91.802	-44.556	-80.265
-3	9	9	48.774	49.523	-47.926	-12.475
-3	9	8	108.436	106.605	-100.357	-35.959
-3	9	7	34.930	25.533	-10.085	23.457
-3	9	6	40.577	29.548	-26.435	-13.202
-3	9	5	17.844	24.409	-8.462	-22.896
-3	9	4	80.475	83.913	-64.493	53.685
-3	9	3	64.784	79.983	-34.238	-72.285
-3	9	2	40.025	46.088	-14.972	43.589
-3	9	1	125.439	127.475	-43.215	-119.926
-3	11	13	63.828	66.104	-31.991	-57.848
-3	11	12	39.657	39.322	-39.164	3.521
-3	11	11	75.738	73.680	-60.222	-42.451
-3	11	10	56.393	55.192	-27.680	47.749
-3	11	9	47.770	43.594	-20.368	-38.544
-3	11	8	58.767	40.517	3.703	40.348
-3	11	7	85.583	73.428	-62.698	-38.218
-3	11	6	51.607	44.128	-43.639	-6.553
-3	11	5	93.099	85.780	-68.983	-50.986
-3	11	4	14.625 *	26.200	-10.088	-24.180
-3	11	3	46.081	58.656	-34.141	47.696
-3	11	2	49.352	50.300	-37.369	-33.670

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-3	11	1	28.040		36.228	-24.043	27.099
-3	13	10	55.610		42.640	-17.356	-38.948
-3	13	9	46.664		46.089	-45.920	3.939
-3	13	8	93.017		90.393	-70.284	-56.843
-3	13	7	52.924		40.098	-5.394	39.733
-3	13	6	8.144	*	11.875	8.225	-8.565
-3	13	5	37.529		31.123	-31.100	1.208
-3	13	4	25.815		20.892	-20.527	-3.892
-3	13	3	0.0	*	3.310	1.253	-3.064
-3	13	2	23.991		14.796	-13.190	6.705
-3	13	1	94.341		94.766	-70.308	-63.540
-3	15	5	30.536		33.748	-33.219	-5.951
-3	15	4	40.792		43.070	-33.827	-26.659
-3	15	3	9.760	*	15.017	9.701	11.463
-3	15	2	17.757	*	18.002	-12.631	-12.827
-3	15	1	28.328		29.268	6.974	28.424
-2	14	8	68.852		69.690	-49.875	48.674
-2	14	7	74.194		79.205	-78.220	-12.454
-2	14	6	32.266		32.730	-17.488	-27.666
-2	14	5	70.556		70.278	-65.881	-24.469
-2	14	4	28.483		15.197	-14.961	2.671
-2	14	3	83.129		74.901	-72.001	-20.639
-2	14	2	35.012		29.198	-29.150	1.664
-2	14	1	100.396		90.021	-89.532	9.371
-2	12	12	29.370		34.165	-30.880	14.616
-2	12	11	73.373		70.283	-67.276	20.337
-2	12	10	45.314		54.279	-47.013	-27.129
-2	12	9	51.341		36.241	-34.432	-11.309
-2	12	8	61.360		72.541	-72.152	-7.507
-2	12	7	30.032		20.732	-12.251	-16.725
-2	12	6	89.538		94.140	-93.809	7.890
-2	12	5	60.923		55.891	-50.190	24.592
-2	12	4	136.940		141.072	-136.427	35.901
-2	12	3	23.714		33.482	-19.635	-27.120
-2	12	2	116.165		105.907	-102.769	-25.589
-2	12	1	37.470		51.221	-51.022	4.508
-2	10	14	81.685		80.432	-73.586	-32.472
-2	10	13	56.764		51.539	38.696	-34.042
-2	10	12	87.121		82.365	-82.343	-1.931
-2	10	11	33.703		35.697	-34.715	8.314
-2	10	10	85.242		71.407	-69.420	-16.729
-2	10	9	13.554	*	37.753	-37.718	-1.620
-2	10	8	105.486		96.089	-92.173	27.153
-2	10	7	104.252		121.211	-120.150	16.006
-2	10	6	77.837		80.804	-14.557	-79.482
-2	10	5	85.217		91.831	-91.799	-2.400
-2	10	4	30.275		22.065	-20.806	-7.349
-2	10	3	133.307		128.481	-128.301	-6.798
-2	10	2	44.580		41.211	-22.271	-34.675
-2	10	1	163.127		155.212	-149.612	41.317
-2	8	16	35.712		39.341	26.390	-29.176
-2	8	15	86.107		85.859	-85.743	-4.446
-2	8	14	15.869	*	23.985	11.654	20.964

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-2	8	13	125.870		122.486	-122.434	-3.563
-2	8	12	14.992	*	28.246	-22.879	-16.564
-2	8	11	118.200		116.128	-115.079	15.569
-2	8	10	25.342		28.154	-10.306	-26.200
-2	8	9	100.085		88.374	-82.546	-31.563
-2	8	8	67.929		82.316	-75.302	-33.250
-2	8	7	39.369		31.677	-30.954	6.726
-2	8	6	93.656		99.690	-99.464	-6.700
-2	8	5	101.420		99.313	-98.365	13.686
-2	8	4	195.881		207.344	-206.613	-17.398
-2	8	3	37.311		30.933	-8.891	-29.627
-2	8	2	135.959		128.407	-125.462	-27.343
-2	8	1	68.333		76.037	-75.731	-6.809
-2	6	17	5.444	*	19.056	-3.095	18.803
-2	6	16	113.219		116.996	-116.938	-3.689
-2	6	15	33.482		29.602	-25.290	-15.385
-2	6	14	91.597		90.650	-90.106	9.911
-2	6	13	61.363		57.021	48.372	-30.193
-2	6	12	140.384		133.785	-133.406	10.065
-2	6	11	33.291		41.528	-34.696	-22.821
-2	6	10	110.200		105.046	-100.840	29.427
-2	6	9	65.497		78.145	-72.088	-30.167
-2	6	8	135.669		134.465	-121.519	57.567
-2	6	7	175.900		192.728	-189.328	-36.043
-2	6	6	13.174	*	7.550	-0.937	-7.492
-2	6	5	150.999		164.343	-156.588	-49.889
-2	6	4	31.191		33.334	-12.439	30.926
-2	6	3	226.141		226.550	-226.537	-2.477
-2	6	2	33.735		47.244	-47.185	-2.354
-2	6	1	227.675		220.447	-219.288	22.577
-2	4	18	26.533		34.791	-28.735	19.613
-2	4	17	81.048		74.737	-72.673	-17.445
-2	4	16	20.330		20.139	8.663	-18.181
-2	4	15	65.823		67.510	-66.473	-11.790
-2	4	14	30.934		37.521	-14.006	34.808
-2	4	13	207.397		206.851	-206.550	-11.157
-2	4	12	39.720		41.014	-34.418	-22.306
-2	4	11	88.935		89.539	-89.528	-1.363
-2	4	10	53.488		52.912	-50.904	14.437
-2	4	9	155.857		152.279	-145.083	-46.259
-2	4	8	135.241		142.850	-142.445	-10.753
-2	4	7	44.180		49.382	49.346	-1.866
-2	4	6	276.618		286.088	-285.880	10.903
-2	4	5	90.527		86.294	-86.264	2.267
-2	4	4	336.287		353.294	-352.859	-17.539
-2	4	3	55.944		47.019	37.712	-28.082
-2	4	2	266.294		264.605	-264.476	-8.288
-2	4	1	102.572		112.267	-104.305	-41.525
-2	2	18	71.127		56.548	-53.557	-18.147
-2	2	17	29.110		22.991	-8.573	21.333
-2	2	16	150.568		143.275	-139.470	-32.800
-2	2	15	23.065		20.485	-6.044	19.574
-2	2	14	116.409		116.832	-115.832	-15.253

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-2	2	13	32.805		36.333	33.887	-13.107
-2	2	12	114.597		119.264	-117.429	-20.839
-2	2	11	45.299		43.116	-38.294	19.813
-2	2	10	182.090		187.115	-187.032	-5.561
-2	2	9	99.581		89.680	-89.651	-2.275
-2	2	8	60.918		69.432	-62.599	-30.036
-2	2	7	280.151		278.083	-276.933	25.264
-2	2	6	50.350		63.706	-54.984	-32.175
-2	2	5	204.680		206.650	-206.155	-14.294
-2	2	4	95.380		97.622	97.146	9.624
-2	2	3	412.571		439.023	-438.868	11.668
-2	0	18	23.370	*	17.108	17.107	0.096
-2	0	17	120.462		114.370	-113.734	-12.038
-2	0	16	58.820		51.220	50.829	6.313
-2	0	15	84.622		86.952	-85.321	-16.761
-2	0	14	24.227	*	16.932	16.141	5.112
-2	0	13	226.711		240.112	-238.944	-23.663
-2	0	12	18.756	*	41.641	41.581	2.238
-2	0	11	113.660		128.386	-127.164	-17.670
-2	0	9	187.704		196.101	-195.790	-11.026
-2	0	8	29.136		35.460	34.688	-7.358
-2	0	7	48.025		49.552	-49.361	-4.343
-2	0	6	313.061		300.157	-299.540	-19.242
-2	0	5	34.060		42.331	-42.172	-3.676
-2	0	4	238.400		224.479	-223.296	-23.012
-2	0	3	36.260		46.389	-46.387	-0.458
-2	0	1	5.020	*	9.952	-9.866	-1.300
-1	1	18	62.230		60.897	45.454	-40.526
-1	1	17	70.275		76.234	57.735	49.782
-1	1	16	85.975		97.657	28.646	-93.361
-1	1	15	23.863		33.885	16.229	29.746
-1	1	14	70.730		77.848	70.935	-32.072
-1	1	13	75.792		85.990	70.128	49.764
-1	1	12	68.934		53.382	14.757	51.301
-1	1	11	55.274		55.308	49.342	-24.988
-1	1	10	110.093		101.607	44.942	91.127
-1	1	9	188.190		173.806	79.168	-154.729
-1	1	8	95.461		85.010	10.373	84.375
-1	1	7	233.347		221.877	83.460	-205.582
-1	1	6	162.331		157.031	2.617	157.009
-1	1	5	93.539		95.668	83.367	-46.928
-1	1	4	217.638		213.545	36.445	210.412
-1	1	3	84.808		101.739	62.107	-80.583
-1	1	2	41.224		34.600	8.830	-33.454
-1	1	1	54.378		39.304	17.752	-35.067
-1	3	18	81.638		92.973	46.925	80.262
-1	3	17	75.638		75.829	49.788	-57.194
-1	3	16	79.173		92.301	29.927	87.315
-1	3	15	45.026		45.390	31.341	-32.833
-1	3	14	98.006		104.370	72.114	75.450
-1	3	13	87.542		85.099	8.561	-84.668
-1	3	12	59.333		50.676	32.643	-38.761
-1	3	11	32.934		31.024	25.387	17.833

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-1	3	10	106.736		104.710	98.481	-35.576
-1	3	9	69.585		74.371	13.124	73.204
-1	3	8	68.909		68.727	45.054	-51.900
-1	3	7	152.104		153.903	34.970	149.878
-1	3	6	146.901		149.442	64.256	-134.923
-1	3	5	44.789		45.226	-21.641	39.712
-1	3	4	158.347		150.867	21.171	-149.375
-1	3	3	24.477		29.890	2.447	-29.790
-1	3	2	72.555		70.794	37.559	-60.010
-1	3	1	69.049		51.714	44.398	26.516
-1	5	17	55.498		54.294	0.836	54.287
-1	5	16	95.021		95.749	48.503	-82.554
-1	5	15	62.858		71.847	51.170	50.435
-1	5	14	40.225		42.666	30.066	-30.272
-1	5	13	46.976		50.856	28.131	42.366
-1	5	12	90.338		79.436	69.362	38.717
-1	5	11	94.227		102.808	94.348	40.838
-1	5	10	41.544		41.580	28.272	30.489
-1	5	9	114.259		117.185	-44.313	-108.483
-1	5	8	112.855		117.162	76.543	88.702
-1	5	7	97.054		100.933	73.936	-68.709
-1	5	6	52.053		45.417	38.910	23.425
-1	5	5	46.313		44.370	32.094	-30.637
-1	5	4	215.766		212.245	92.229	191.159
-1	5	3	42.639		57.575	55.498	15.322
-1	5	2	36.283		57.100	1.115	-57.089
-1	5	1	62.986		64.559	-62.448	16.375
-1	7	16	65.093		69.119	29.567	62.476
-1	7	15	52.986		48.870	48.848	1.466
-1	7	14	71.322		70.539	44.662	54.599
-1	7	13	53.588		47.053	16.090	-44.216
-1	7	12	27.380		26.358	20.076	-17.079
-1	7	11	56.072		57.295	29.700	48.996
-1	7	10	56.004		65.555	35.126	-55.350
-1	7	9	111.523		120.176	89.485	80.217
-1	7	8	44.472		45.654	35.790	-28.344
-1	7	7	178.842		182.884	44.489	177.390
-1	7	6	117.551		111.302	3.821	-111.237
-1	7	5	55.822		42.098	30.484	29.035
-1	7	4	55.363		43.276	10.962	-41.865
-1	7	3	68.550		47.783	-1.545	47.758
-1	7	2	65.096		45.118	14.593	-42.693
-1	7	1	149.929		138.304	125.474	58.174
-1	9	15	29.564		43.915	42.160	12.293
-1	9	14	17.823	*	9.013	-5.633	-7.036
-1	9	13	65.364		63.748	59.802	22.081
-1	9	12	60.559		59.784	57.008	18.006
-1	9	11	45.585		56.413	56.411	0.508
-1	9	10	59.960		70.724	-23.520	66.699
-1	9	9	84.562		92.491	14.539	-91.341
-1	9	8	69.667		69.852	43.825	54.394
-1	9	7	89.857		97.530	24.668	-83.982
-1	9	6	68.137		57.223	-6.394	56.864

JOAQUINITE - STRUCTURE FACTORS

H	K	L	F(OBS)		F(CALC)	A(CALC)	B(CALC)
-1	9	5	67.260		54.392	37.122	-39.755
-1	9	4	127.844		110.922	79.496	77.356
-1	9	3	51.745		40.105	38.611	-10.844
-1	9	2	41.026		35.165	-33.571	10.466
-1	9	1	56.595		47.997	-35.168	-32.664
-1	11	13	27.700		9.787	3.523	-9.131
-1	11	12	18.717	*	22.262	10.079	-19.850
-1	11	11	17.489	*	20.945	-19.371	-7.966
-1	11	10	58.540		57.453	57.403	2.392
-1	11	9	63.123		69.397	49.981	48.144
-1	11	8	49.713		54.190	32.892	-43.066
-1	11	7	57.098		55.348	-13.496	53.678
-1	11	6	48.506		45.447	45.437	0.980
-1	11	5	37.916		26.807	13.711	23.036
-1	11	4	76.199		65.816	-31.009	-58.053
-1	11	3	0.0	*	25.807	-23.582	-10.482
-1	11	2	48.589		53.584	52.531	10.567
-1	11	1	46.156		35.623	35.250	5.145
-1	13	10	6.786	*	26.511	5.579	25.917
-1	13	9	18.068	*	7.487	-5.913	-4.593
-1	13	8	16.031	*	13.600	13.229	3.154
-1	13	7	29.118		31.959	8.291	-30.865
-1	13	6	50.820		47.858	36.306	31.181
-1	13	5	21.944		12.081	11.096	-4.778
-1	13	4	51.450		39.998	36.539	16.272
-1	13	3	31.136		34.280	30.245	16.136
-1	13	2	31.076		23.317	15.485	17.433
-1	13	1	45.903		46.297	-46.290	0.832
-1	15	5	42.596		31.338	24.735	19.242
-1	15	4	58.180		48.964	-43.618	-22.248
-1	15	3	32.079		8.092	2.925	7.545
-1	15	2	40.430		40.958	40.902	2.141
-1	15	1	51.581		43.104	43.097	0.781