

## Crystal Structure of Joaquinite

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### Abstract

The crystal structure of monoclinic joaquinite, ideal formula  $\text{NaFe}^{2+}\text{Ba}_2\text{RE}_2\text{Ti}_2\text{Si}_3\text{O}_{26}\text{OH}\cdot\text{H}_2\text{O}$ , 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  $a = 10.516 \pm 0.003 \text{ \AA}$ ,  $b = 9.686 \pm 0.003 \text{ \AA}$ ,  $c = 11.833 \pm 0.004 \text{ \AA}$ , and  $\beta = 109.67 \pm 0.003^\circ$ , 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,  $\text{H}_2\text{O}$ ). The principal structural unit is a four-membered  $\text{Si}_4\text{O}_{12}$  silicate ring, equivalents of which are linked by  $\text{TiO}_6$  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- $\text{H}_2\text{O}$  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  $\text{H}_2\text{O}$ . Macroscopic twinning of the monoclinic form on this plane and disordered stacking of monoclinic and orthorhombic forms also occur.

### Introduction

Joaquinite occurs as small ( $\sim 1 \text{ mm}$ ) honey-brown crystals associated with benitoite, neptunite, and natrolite in San Benito County, California (Loudersback 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  $\text{NaBa}_2\text{Fe}^{2+}\text{Ce}_2\text{Ti}_2\text{Si}_3\text{O}_{26}\text{OH}$  for joaquinite from Greenland, and Laird and Albee (1972) suggested the formula  $\text{Ba}_{8.1}(\text{Sr}_{1.7}\text{RE}_{6.5}\text{Th}_{0.1})_{8.3}(\text{Ca}_{0.2}\text{Na}_{3.3}\text{Fe}_{3.1}\text{Li}_{0.3}\text{Mg}_{0.1})_{7.5}\text{Ti}_{8.1}\text{Si}_{32.0}\text{O}_{98.7}(\text{OH})_{13.3}$  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	40.802
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	69.328	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	-18.589
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	5	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	0.922	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	139.141	31.814
0	8	5	136.500	116.327	116.273	-0.546
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	95.068	81.043	82.452	2.885

## 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	19.459	-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	-10.564
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	53.223	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	9.562	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	-55.865
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	29.898	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	37.232	37.273	-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	87.286
1	7	7	101.099	103.815	86.626	57.215
1	7	8	24.051	30.468	-27.711	12.657
1	7	9	55.077	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	65.290	-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	120.018
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	-1.910
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	-39.437	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	8	176.402	175.327	-174.029	-21.288
2	0	9	28.260	38.157	38.127	-1.509
2	0	10	167.585	176.165	-175.264	-17.796
2	0	11	114.764	131.811	-131.464	-9.562
2	0	12	62.327	50.670	-50.290	-6.198
2	0	13	16.280 *	28.378	-26.237	-10.813
2	0	14	33.522	11.212	-11.130	1.358
2	0	15	104.122	119.123	-118.116	-15.457
2	0	16	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	25.859	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	78.836	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
2	2	17				

## 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	48.998	49.175	-48.910	-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	-14.691	-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	21.073	24.180	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	85.820	-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	279.790	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 *	14.792	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	-13.252
4	2	7	44.564	37.342	-36.853	.023
4	2	9	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	-3.187
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	22.469	-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	39.888	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	52.108
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	6.353	-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	-25.689	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	129.090	-128.372	-13.671
6	2	6	111.679	109.071	-105.757	-26.705
6	2	7	177.661	198.128	-185.726	29.968
6	2	8	17.556 *	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	-43.402	-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	-116.308	-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	-38.425	-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	30.762
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	-31.238	-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 *	26.955	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	122.614	132.852	120.397	56.161

## JOAQUINITE - STRUCTURE FACTORS

H	K	L	F (OBS)	F (CALC)	A (CAIC)	B (CAIC)
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	68.836	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	35.287	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	11.73
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 *	3.707	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	87.114	83.526	44.307	-70.806
9	7	1	83.074	81.755	69.490	43.069
9	7	2	46.162	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 (CALC)	B (CALC)
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	144,024	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	0	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	112.331	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	45.177
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	113.012	113.274	113.251	-5.277

## JACQUINITE - 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	39.792	-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	-53.969	-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	63.303	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	31.623	31.416	-4.216	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	22.675		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	46.090	-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	85.302	80.203	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 *	16.589	-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	51.542	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	91.023	-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	96.825	-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	68.349	-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	-20.582	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	81.128	-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	62.583	-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	23.723
-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	80.038		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	14.535
-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	-48.615



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	45.669	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

## JOAQUINITE - 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	-3.050
-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	76.770	-27.756
-8	10	5	9.573 *	5.273	4.445	2.839
-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	27.286	20.205	-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	-26.546	-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	115.139	122.710	-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)	E (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	15.527
-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	-1.640	-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	7.663
-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	22.655	16.712	16.578	-2.113
-6	2	9	195.670	198.463	-195.146	36.132
-6	2	8	36.776	34.891	-31.895	-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	63.659	-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	-79.698	-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(CAIC)	A(CAIC)	B(CAIC)
-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	102.340	100.931	60.030	79.620

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 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	18.339
-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 (CALC)	A (CALC)	B (CALC)
-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	15.379	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	156.529	5.352
-4	8	3	73.444	102.013	99.115	-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	77.657	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	26.664	-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	69.684	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

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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	93.523	-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	-14.977	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	6.574	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	15.157	-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	-85.742	-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	-206.612	-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	89.538	-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	32.024	31.024	25.367	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	80.338	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	73.926	-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	87.857	97.530	24.668	-83.982
-1	9	6	55.322	55.322	-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