

The crystal structures of high albite and monalbite at high temperatures

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Abstract

X-ray diffraction data obtained at 24, 300, 600, 750, 900, 1090, and 1105°C have been used to investigate the crystal structure of high albite at high temperatures. These results show that, for the models tested, splitting of Na into four quarter-atoms gives the best agreement between the structure model and X-ray intensities. At high temperatures, albite twinning and broadened diffraction peaks make detection of the albite-monalbite transition difficult; however, these single crystals of synthetic high albite ($\text{Or}_{0.5}\text{Ab}_{99.3}\text{An}_{1.2}$) were not monoclinic at 1105°C. This contrasts with other investigations where the high albite-monalbite transition has been reported to occur at temperatures as low as 930°C. Possible reasons for these discrepancies include different prior thermal histories, the presence of polysynthetic twinning and/or other defects in crystals transforming at the lower temperatures, different compositions for the crystals, and errors in measurement of the transition point. Although no direct evidence has been found for a domain structure in high albite, a possible explanation for the observations is that four kinds of domains or regions exist in the crystal, each of which contains an ordered triclinic arrangement of AlSi_3 , but with Al occupying a different one of the four possible tetrahedral sites in the crystal structure comprising each region. Each Na position is then a function of the immediate Al/Si environment.

Introduction

Ferguson *et al.* (1958) reported the first refinements of the structures of low albite and high albite. In that paper several questions were raised about the structures which have not yet been answered satisfactorily. These questions involve the nature of the Na atom and the degree of Al/Si disorder in the low- and high-albite structures. These authors found that the Na atom in low albite has an unusually anisotropic thermal vibration which could be interpreted as thermal vibration or as a random occupancy of one of two positions separated by $\sim 0.1\text{\AA}$ in the relatively large cavity in which Na resides. The anisotropic character of Na in high albite was found to be even greater, with a separation for the split atom model of approximately 0.6\AA . The problem was reviewed again by Ribbe *et al.* (1969) using new three-dimensional X-ray data. In their paper the problem and experimental evidence were more clearly defined;

however, the conclusion for low albite was that neither of the possible models could be ruled out by the evidence at hand. For high albite the evidence was again not definitive, but the best match to the data was obtained using a quarter-atom model with four quarter-atoms distributed in an approximate line along the major axis of the anisotropic Na Fourier peak and with separations of 0.9\AA between the outer pair and 0.2\AA between the inner pair. Although there is some discussion of possible domain structures in high albite in Ribbe *et al.* (1969), and although Quarnei and Taylor (1971) reported on a high-temperature study of low albite, the behavior of the Na atom in albite is still not well understood.

With regard to the question of Al/Si ordering in albite, one would like to know whether low albite is completely ordered and high albite completely disordered; also, there is the question of whether intermediate albites exist, and if so, whether the lattice parameters change in a regular way as a function of Al/Si ordering. Ribbe *et al.* (1969) concluded that Al is ordered into one site and Si into the other three

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SUENO, PREWITT, AND PAPKE - HIGH ALBITE - 24 DEG. C

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
2	0	0	6.067	5.931	-7	5	0	2.465	3.023	-1	11	0	19.159	17.972	-4	14	1	1.992	0.945
4	0	0	112.926	115.360	-9	5	0	6.546	6.123	-1	11	0	7.922	5.012	-2	14	1	42.215	12.941
6	0	0	109.623	110.150	-8	6	0	40.943	40.034	-3	11	0	21.191	24.034	0	14	1	22.359	24.033
8	0	0	9.069	9.215	-6	6	0	14.553	13.855	-5	11	0	23.143	19.339	-2	14	1	4.993	3.012
10	0	0	57.051	57.150	-4	6	0	44.420	44.010	-7	11	0	5.161	7.804	4	14	1	45.102	45.124
9	1	0	3.146	4.038	-2	6	0	83.317	33.010	-6	12	0	3.273	0.733	5	13	1	11.638	10.139
7	1	C	36.523	35.745	0	6	C	94.446	30.433	-4	12	0	6.968	0.533	4	0	0	112.826	115.355
5	1	0	10.027	12.200	2	6	0	78.687	11.143	-2	12	0	43.664	41.120	3	13	1	16.394	15.394
3	1	0	44.380	45.386	4	0	0	112.826	115.355	0	12	0	19.944	17.971	1	13	1	21.543	22.244
1	1	0	10.316	9.124	4	6	0	72.279	11.213	-2	12	0	36.142	33.093	-1	13	1	25.833	25.297
-1	1	0	27.489	23.449	6	6	0	24.949	25.071	4	12	0	23.772	25.440	-3	13	1	6.338	5.054
-3	1	0	46.112	48.030	8	6	0	35.508	34.997	6	12	0	23.385	22.437	-5	13	1	3.215	0.734
-5	1	0	13.675	13.750	9	7	0	13.381	13.023	5	13	0	19.413	17.550	-7	13	1	23.316	24.020
-7	1	0	45.287	45.557	7	7	0	14.460	10.231	3	13	0	27.732	20.709	-8	12	1	18.628	17.333
-9	1	0	10.114	9.975	5	7	0	31.565	32.132	1	13	0	23.974	23.551	-6	12	1	14.674	15.214
-3	2	0	26.716	23.737	3	7	0	38.775	33.124	2	13	0	6.875	3.035	-4	12	1	58.777	55.275
-6	2	0	42.036	43.733	1	7	0	16.054	3.073	-3	13	C	12.047	13.568	-2	12	1	11.349	10.330
-4	2	C	42.019	40.252	-1	7	0	62.258	33.137	-5	13	0	30.289	27.074	0	12	1	9.023	14.024
-2	2	0	117.462	119.471	-3	7	0	28.032	29.112	4	0	C	112.826	115.355	2	12	1	45.552	45.933
4	0	C	113.219	119.366	-5	7	C	21.572	22.043	-7	13	0	22.946	20.537	4	12	1	28.153	27.112
0	2	0	31.317	31.550	-7	7	0	23.143	23.703	-6	14	0	13.525	12.042	6	12	1	24.572	25.550
2	2	C	111.533	111.184	-9	7	0	5.663	4.830	-4	14	C	37.453	30.440	7	11	1	8.636	3.033
4	2	C	60.111	59.033	-8	8	0	35.779	33.054	-2	14	0	19.599	17.912	5	11	1	10.223	3.000
6	2	0	65.029	65.932	-6	8	0	10.518	5.570	0	14	0	40.547	37.131	3	11	1	23.673	23.393
3	2	0	27.166	25.074	-4	8	0	21.526	23.075	2	14	0	10.064	8.512	1	11	1	17.061	17.360
9	3	0	38.850	33.729	-2	8	0	110.604	113.219	4	14	0	4.335	2.710	-3	11	1	21.509	21.350
7	3	0	17.104	17.540	0	8	0	57.253	54.423	5	15	0	11.505	11.912	4	0	0	112.826	115.350
5	3	0	50.759	49.721	2	8	C	58.885	50.525	3	15	0	22.606	21.117	-5	11	1	15.332	15.520
3	3	0	29.452	32.004	4	8	0	53.443	50.032	1	15	0	18.311	19.243	-7	11	1	9.715	11.230
1	3	0	92.270	39.942	4	0	0	112.826	115.355	-1	15	C	12.163	11.871	-8	10	1	5.924	5.287
-1	5	0	107.931	105.351	6	8	0	6.182	2.033	-5	15	0	7.285	3.239	-6	10	1	16.354	16.133
-3	3	0	18.953	22.043	8	8	0	68.169	53.523	-4	16	0	11.083	13.431	-4	10	1	24.395	22.312
-5	3	0	38.278	37.920	7	9	0	24.049	24.254	-2	16	C	11.840	11.029	-2	10	1	48.040	47.333
-7	3	0	27.645	27.939	5	9	0	49.368	49.040	0	16	0	24.430	24.303	2	10	1	19.696	19.335
-9	2	0	31.218	31.973	3	9	0	8.913	9.911	2	16	0	14.241	11.012	4	10	1	16.529	19.235
-8	4	C	35.981	37.050	1	9	C	85.389	83.732	4	16	0	4.306	4.032	6	10	1	17.947	16.134
-6	4	0	83.640	80.200	-1	9	0	38.844	35.772	-1	17	0	7.424	6.449	7	9	1	12.434	11.339
-4	4	0	24.447	23.031	-3	9	0	6.962	4.125	-1	17	C	18.426	17.211	5	9	1	21.186	21.431
-2	4	C	47.653	45.719	-5	9	0	45.783	30.021	4	0	0	112.826	115.355	3	9	1	30.023	28.318
0	4	3	143.121	150.825	-7	9	0	4.179	5.710	-3	17	0	19.685	20.705	-1	9	1	63.285	53.352
4	0	0	112.901	115.355	-8	10	0	15.142	17.170	1	17	1	40.065	33.059	-3	9	1	46.002	45.206
2	4	C	65.479	65.377	-6	10	0	4.283	0.936	-1	17	1	7.452	8.038	-7	9	1	47.549	45.043
4	4	0	7.869	7.233	-6	10	0	17.179	15.300	-3	17	1	34.064	32.620	-9	9	1	6.240	4.032
0	4	C	82.191	82.437	-2	10	0	35.923	35.510	-4	16	1	10.587	8.333	-8	8	1	27.016	21.727
8	4	0	45.056	44.733	0	10	0	45.881	51.131	-2	16	1	32.540	32.137	4	0	0	112.826	115.355
9	5	0	6.142	5.621	-2	10	0	15.032	13.525	0	16	1	23.585	24.530	-6	8	1	7.320	8.243
7	5	0	25.319	21.533	4	10	C	2.800	3.033	2	16	1	7.787	9.132	-4	8	1	77.746	77.721
5	5	0	30.970	29.032	6	10	0	21.174	21.058	3	15	1	13.375	13.123	-2	8	1	23.489	17.739
3	5	0	5.005	5.093	8	10	0	2.257	4.934	1	15	1	34.301	35.079	0	8	1	19.838	19.933
1	5	C	13.791	2.913	7	11	0	28.078	29.233	-1	15	1	12.613	11.531	2	8	1	69.693	59.933
-1	5.	0	29.602	23.712	4	0	0	112.826	115.355	-3	15	1	43.503	42.011	4	8	1	21.803	23.373
-3	5	0	7.539	5.007	5	11	C	18.155	17.039	-5	15	1	21.445	22.030	6	8	1	32.950	34.333
-5	5	0	45.587	43.744	3	11	0	14.755	15.030	-6	14	1	44.796	43.226	8	8	1	5.057	2.721

SUENO, PREWITT, AND PARKE - H-H ALBITE - 24 DEG. C

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
7	7	1	12.261	10.013	0	2	1	15.292	15.030	-3	-3	1	75.189	70.210	3	-9	1	7.071	9.037
5	7	1	5.138	2.033	2	2	1	42.111	42.003	-5	-3	1	46.666	47.015	1	-9	1	75.933	74.033
3	7	1	21.301	21.312	4	2	1	3.221	3.030	-7	-3	1	26.941	27.003	-1	-9	1	13.520	1.0310
1	7	1	32.165	32.002	6	2	1	5.986	5.033	-9	-3	1	24.309	24.705	-3	-9	1	5.502	5.0313
-1	7	1	35.998	33.471	8	2	1	7.764	7.035	-10	-4	1	20.325	21.302	-5	-9	1	27.813	26.657
-3	7	1	7.412	1.030	9	1	1	26.444	27.030	-8	-4	1	34.105	32.470	-7	-9	1	24.499	23.0326
-5	7	1	44.201	44.494	7	1	1	34.780	35.033	-6	-4	1	1.445	1.713	-6	-10	1	1.357	2.023
-7	7	1	18.524	20.411	5	1	1	15.956	15.249	-4	-4	1	50.811	49.611	-4	-10	1	16.510	14.035
-9	7	1	17.237	15.003	3	1	1	35.235	33.033	4	0	0	112.826	110.300	-2	-10	1	11.101	3.209
-10	6	1	35.265	35.055	1	1	1	85.522	87.700	-2	-4	1	117.104	110.327	0	-10	1	37.897	39.210
-8	6	1	29.013	24.709	-1	1	1	28.032	27.375	0	-4	1	92.333	94.311	2	-10	1	29.810	33.032
-6	6	1	11.170	12.504	-3	1	1	6.569	6.997	2	-4	1	103.359	99.424	4	-10	1	5.109	4.373
-4	0	0	112.826	113.010	-5	1	1	48.600	49.734	4	-4	1	39.444	40.003	6	-10	1	27.293	24.455
-4	6	1	107.896	107.119	-7	1	1	17.220	18.021	6	-4	1	51.394	52.000	7	-11	1	26.127	20.039
-2	6	1	21.168	17.032	-9	1	1	27.253	23.074	8	-4	1	32.760	34.019	4	0	0	112.826	112.000
-0	6	1	73.723	73.207	-10	0	1	6.849	8.391	9	-5	1	13.185	11.436	5	-11	1	11.049	13.003
2	6	1	30.924	31.033	-8	0	1	56.768	53.037	7	-5	1	21.209	21.001	3	-11	1	33.095	31.033
4	6	1	10.091	10.124	-6	0	1	25.689	28.751	5	-5	1	10.323	3.039	1	-11	1	19.517	21.033
6	6	1	30.381	33.701	-4	0	1	54.505	51.133	3	-5	1	48.375	57.595	-1	-11	1	10.737	7.703
8	6	1	2.534	5.033	4	0	0	112.826	113.000	1	-5	1	40.212	42.032	-3	-11	1	40.563	42.030
7	5	1	13.565	13.033	-2	0	1	141.811	110.207	-1	-5	1	47.313	49.120	-5	-11	1	15.465	17.034
5	5	1	8.197	8.353	0	0	1	21.168	21.700	-3	-5	1	31.542	27.995	-7	-11	1	2.563	3.033
3	5	1	72.003	70.321	2	0	1	7.776	5.253	-5	-5	1	35.779	41.250	-6	-12	1	16.446	15.232
1	5	1	66.264	50.312	4	0	1	31.149	32.213	-7	-5	1	31.386	31.730	-4	-12	1	10.171	0.034
-1	5	1	40.876	42.333	6	0	1	49.454	50.704	-9	-5	1	8.601	9.020	-2	-12	1	54.950	51.034
-3	5	1	34.636	32.092	8	0	1	20.908	20.200	-8	-6	1	5.138	5.501	0	-12	1	34.901	30.033
-5	5	1	32.621	32.144	9	-1	1	28.938	29.369	-6	-6	1	2.748	3.003	2	-12	1	50.615	49.033
-7	5	1	41.424	41.524	7	-1	1	30.220	31.070	-4	-6	1	43.462	39.258	4	-12	1	23.477	21.034
-9	5	1	11.522	11.704	5	-1	1	21.284	21.044	-2	-6	1	17.012	15.303	6	-12	1	17.699	17.129
-8	4	1	19.223	19.709	3	-1	1	35.225	32.700	4	0	0	112.826	110.300	5	-13	1	19.575	20.033
-6	4	1	67.188	53.033	-1	-1	1	70.883	72.521	2	-6	1	29.608	28.401	3	-13	1	22.871	23.030
-4	4	1	62.229	51.073	-1	-1	1	25.769	23.713	4	-6	1	33.008	33.017	1	-13	1	21.746	23.031
4	0	0	112.826	110.300	-3	-1	1	4.970	5.031	8	-6	1	21.774	21.013	-1	-13	1	5.952	0.727
-2	4	1	99.647	90.030	-5	-1	1	31.669	31.434	5	-7	1	30.439	32.400	-3	-13	1	12.960	14.037
0	4	1	14.870	9.030	-7	-1	1	9.635	10.150	3	-7	1	10.997	9.001	-5	-13	1	25.567	21.031
2	4	1	27.247	24.070	-9	-1	1	18.501	19.030	1	-7	1	26.442	27.710	4	0	0	112.826	113.000
-4	4	1	65.860	69.313	-10	-2	1	17.576	19.320	-1	-7	1	35.392	32.266	-7	-13	1	18.830	21.540
6	4	1	36.421	35.412	-8	-2	1	22.282	23.932	-3	-7	1	20.712	19.831	-6	-14	1	20.799	20.414
8	4	1	19.708	18.041	-6	-2	1	35.558	35.175	-5	-7	1	12.140	10.500	-4	-14	1	26.964	29.032
7	3	1	27.680	23.030	-4	-2	1	7.770	8.023	-7	-7	1	5.282	4.509	-2	-14	1	10.575	5.303
5	3	1	27.455	21.033	4	0	0	112.826	113.000	-9	-7	1	24.759	23.934	0	-14	1	35.173	37.035
3	3	1	28.217	29.331	-2	-2	1	26.912	26.022	-8	-8	1	33.718	33.531	2	-14	1	10.472	9.034
1	3	1	95.664	91.350	0	-2	1	17.254	17.333	-6	-8	1	15.580	15.132	4	-14	1	15.794	10.329
-1	3	1	12.382	7.430	2	-2	1	32.206	31.711	-4	-8	1	16.146	9.145	5	-15	1	14.882	13.000
-3	3	1	60.243	59.245	4	-2	1	22.837	22.013	-2	-8	1	101.610	102.034	3	-15	1	40.541	43.032
-5	3	1	42.585	42.133	6	-2	1	13.364	13.334	0	-8	1	53.230	53.327	-1	-15	1	29.071	23.039
-7	3	1	6.194	7.022	8	-2	1	18.501	18.594	2	-8	1	65.173	50.003	-1	-15	1	23.177	23.035
-9	3	1	19.800	19.704	9	-3	1	9.040	9.334	4	0	0	112.826	113.000	-3	-15	1	28.095	23.032
-10	2	1	29.712	31.523	7	-3	1	18.103	13.291	4	-8	1	57.363	55.821	-5	-15	1	1.726	0.305
-6	2	1	34.705	35.632	5	-3	1	9.277	8.420	6	-8	1	12.677	10.728	-4	-16	1	8.353	7.030
-4	2	1	7.603	8.037	3	-3	1	27.518	23.003	8	-8	1	61.155	59.439	-2	-16	1	19.165	10.035
4	0	0	112.826	113.000	-1	-3	1	81.602	31.027	7	-9	1	30.861	30.335	0	-16	1	43.324	43.032
-2	2	1	9.958	9.033	-1	-3	1	50.441	49.030	5	-9	1	29.752	26.408	2	-16	1	5.351	5.031

SUENO, PREWITT, AND FAFIKE - HIGH ALBITE - 24 DEG. C

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-4	-15	1	1.051	1.053	3	-9	2	41.050	40.221	6	-4	2	9.034	10.031	-6	2	2	10.956	7.237
-1	-17	1	24.049	25.053	1	-9	2	15.783	12.019	8	-4	2	8.676	8.013	-4	2	2	102.314	50.373
4	0	0	112.826	115.350	-1	-9	2	105.668	104.985	7	-3	2	46.425	40.324	-2	2	2	20.372	21.057
-3	-17	1	38.864	39.153	-3	-9	2	35.329	34.503	5	-3	2	2.909	3.053	0	2	2	13.225	15.950
1	-17	2	43.399	45.023	-5	-9	2	33.412	33.203	3	-3	2	30.745	30.743	2	2	2	87.531	87.033
-3	-17	2	25.565	27.038	-7	-9	2	49.225	42.515	1	-3	2	38.203	42.935	4	2	2	18.057	17.707
-4	-16	2	4.453	4.449	-9	-9	2	4.052	2.431	-1	-3	2	49.102	43.444	6	2	2	47.440	47.262
-2	-16	2	32.806	32.926	-8	-8	2	44.807	40.509	-3	-3	2	20.048	24.334	4	0	0	112.826	115.350
0	-16	2	4.601	4.283	-6	-8	2	17.555	10.839	-5	-3	2	34.053	32.959	8	2	2	15.794	15.720
2	-16	2	5.651	2.114	-4	-8	2	113.952	110.336	-7	-3	2	4.999	2.730	7	3	2	25.434	20.333
3	-15	2	9.946	8.771	-2	-8	2	18.034	13.540	-9	-3	2	34.682	33.739	3	3	2	36.212	38.170
1	-15	2	16.481	17.173	0	-8	2	61.658	60.613	-10	-2	2	8.815	7.075	1	3	2	14.928	12.037
-1	-15	2	39.791	41.753	-2	-8	2	93.269	97.338	-8	-2	2	33.903	34.375	-1	3	2	70.744	71.853
-3	-15	2	22.808	22.035	4	-8	2	16.117	13.230	-6	-2	2	65.392	60.342	-3	3	2	22.588	19.539
-5	-15	2	23.189	23.823	6	-8	2	55.810	51.050	-4	-2	2	62.385	58.313	-5	3	2	20.984	20.075
-6	-14	2	39.144	37.373	7	-7	2	16.521	16.353	-2	-2	2	66.559	63.697	-7	3	2	4.514	4.963
-2	-14	2	44.074	44.092	5	-7	2	3.492	1.251	0	-2	2	71.475	80.502	-9	3	2	19.944	20.839
0	-14	2	25.030	24.953	3	-7	2	4.532	4.030	2	-2	2	63.441	53.208	-10	4	2	16.417	16.036
2	-14	2	12.555	14.192	-1	-7	2	42.729	42.334	6	0	0	112.826	115.366	-8	4	2	9.686	8.513
4	-14	2	52.179	51.243	-1	-7	2	34.191	35.200	4	-2	2	50.597	52.116	-6	4	2	79.264	30.573
5	-13	2	13.155	11.999	-3	-7	2	18.293	19.042	6	-2	2	46.400	42.831	-4	4	2	75.189	76.300
-4	0	0	112.826	115.350	-5	-7	2	21.278	22.727	8	-2	2	11.049	11.733	-2	4	2	40.466	30.352
3	-13	2	12.752	9.513	-7	-7	2	7.787	0.941	7	-1	2	29.071	23.312	0	4	2	34.249	35.353
1	-13	2	35.652	34.5+1	-9	-7	2	15.321	16.515	5	-1	2	13.208	14.054	2	4	2	81.383	88.753
-1	-13	2	24.713	21.476	-10	-6	2	19.916	20.691	3	-1	2	10.651	13.971	-4	4	2	65.941	57.334
-3	-13	2	26.433	23.937	-8	-6	2	14.085	14.232	1	-1	2	38.908	41.179	6	4	2	8.203	3.170
-5	-13	2	15.286	15.711	-6	-6	2	30.353	30.251	-1	-1	2	50.036	53.042	8	4	2	19.743	20.373
-7	-13	2	20.037	19.562	-4	-6	2	44.051	41.773	-3	-1	2	45.448	46.122	-4	0	0	112.926	115.353
-8	-12	2	3.781	2.021	-2	-6	2	52.202	51.771	-5	-1	2	5.121	10.432	5	5	2	51.994	51.431
-6	-12	2	5.490	6.925	4	0	0	112.826	115.353	-7	-1	2	16.394	15.903	3	5	2	12.792	15.810
-4	-12	2	54.165	51.783	0	-6	2	65.791	67.033	-9	-1	2	14.276	13.953	-1	5	2	32.835	35.353
-2	-12	2	5.305	3.530	2	-6	2	53.460	50.329	-10	0	2	13.970	15.109	-1	5	2	23.604	20.320
0	-12	2	38.267	35.353	4	-6	2	17.982	19.533	-8	0	2	5.548	6.110	-3	5	2	15.505	15.112
2	-12	2	34.203	31.373	6	-6	2	37.401	35.469	-6	0	2	127.708	123.379	-5	5	2	38.480	37.353
4	-12	2	10.789	8.073	8	-6	2	26.935	27.077	-4	0	2	58.748	54.823	-7	5	2	27.264	27.100
6	-12	2	38.798	35.500	7	-5	2	10.691	8.689	-2	0	2	158.263	160.353	-9	5	2	9.854	9.370
5	-11	2	42.446	42.135	5	-5	2	61.992	60.222	0	0	2	166.056	164.926	-10	6	2	22.305	23.613
3	-11	2	44.363	42.920	3	-5	2	26.970	27.054	2	0	2	32.142	30.232	-8	6	2	27.714	27.493
1	-11	2	24.332	27.227	1	-5	2	5.195	1.923	4	0	2	128.251	131.228	-6	6	2	10.749	7.990
-1	-11	2	65.185	52.319	-1	-5	2	31.057	34.353	-4	0	0	112.826	115.353	-4	6	2	70.317	59.299
-3	-11	2	27.385	30.247	-3	-5	2	5.698	0.171	6	0	2	11.690	11.300	-2	6	2	51.301	50.347
-5	-11	2	36.616	35.573	-5	-5	2	24.459	24.231	8	0	2	23.027	23.203	0	6	2	57.646	51.027
-7	-11	2	51.082	51.733	-7	-5	2	50.314	49.755	7	1	2	25.607	25.015	2	6	2	82.601	33.452
-8	-10	2	13.214	13.597	-9	-5	2	3.117	1.014	5	1	2	4.075	7.119	4	6	2	27.027	27.933
-6	-10	2	25.273	20.350	-10	-4	2	23.137	24.015	3	1	2	1.761	4.213	6	6	2	23.529	22.003
-4	-10	2	9.542	8.025	-8	-4	2	15.996	19.120	-1	-1	2	4.041	3.503	-8	6	2	36.760	30.325
-2	-10	2	57.288	53.172	-6	-4	2	55.406	53.333	-1	1	2	71.673	72.099	7	7	2	6.004	5.222
0	-10	2	25.602	21.953	-4	-4	2	95.191	94.054	-3	1	2	23.333	27.013	4	0	0	112.826	115.353
-2	-10	2	1.282	3.430	-2	-4	2	11.361	7.033	-5	1	2	14.351	14.409	5	7	2	15.725	15.824
4	-10	2	25.919	23.177	0	-4	2	12.821	10.513	-7	1	2	16.891	15.452	3	7	2	11.205	12.690
6	-10	2	10.783	11.357	4	0	0	112.826	115.353	-9	1	2	19.812	17.513	1	7	2	2.511	3.090
7	-9	2	3.573	3.353	2	-4	2	78.185	77.177	-10	2	2	4.572	6.103	-3	7	2	17.029	17.226
5	-9	2	.44.305	44.031	4	-4	2	58.390	58.050	-8	2	2	39.831	39.403	-5	7	2	8.076	5.111

SUENO, PREWITT, AND FAPINE - HIGH ALBITE - 24 DEG. C

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-3	-3	3	43.612	45.918	3	-9	3	15.523	12.230	-2	-16	4	25.673	25.720	5	-7	4	22.103	23.793
1	-3	3	44.016	44.914	1	-9	3	27.922	23.400	0	-16	4	4.462	7.601	3	-7	4	14.870	16.493
-1	-3	3	18.270	19.300	-1	-9	3	37.199	35.519	-1	-15	4	27.622	27.732	1	-7	4	68.775	72.550
-3	-3	3	21.272	20.151	-3	-9	3	45.521	43.825	-3	-15	4	25.821	25.037	-1	-7	4	2.938	3.162
-5	-3	3	94.487	93.824	-5	-9	3	15.950	13.154	-5	-15	4	3.169	3.039	-3	-7	4	4.508	5.042
-7	-3	3	25.815	25.372	-7	-9	3	15.349	11.030	-6	-14	4	17.757	16.633	-5	-7	4	67.286	69.132
-9	-3	3	12.931	11.201	-9	0	0	112.826	115.366	-4	-14	4	5.726	3.147	-7	-7	4	17.283	13.761
-10	-4	3	4.428	7.612	-9	-9	3	18.986	20.294	-2	-14	4	34.901	34.723	-9	-7	4	16.111	16.289
-8	-4	3	32.708	32.630	-8	-10	3	8.705	4.235	2	-14	4	27.986	20.041	-10	-6	4	14.033	19.173
-6	-4	3	76.216	77.995	-6	-10	3	11.153	11.245	3	-13	4	26.167	25.247	-8	-6	4	16.931	15.333
-4	-4	3	32.696	33.101	-2	-10	3	8.705	6.299	1	-13	4	26.081	20.051	-6	-6	4	26.993	27.222
-2	-4	3	25.515	22.351	0	-10	3	17.791	16.274	4	0	0	112.826	115.366	-4	-6	4	47.093	44.899
0	-4	3	58.511	60.034	-4	-10	3	6.304	6.032	-1	-13	4	9.536	9.493	-2	-6	4	43.576	43.053
2	-4	3	91.935	93.533	5	-11	3	13.127	15.110	-3	-13	4	8.855	8.010	0	-6	4	56.318	55.759
4	-4	3	41.355	41.780	3	-11	3	4.595	4.592	-5	-13	4	36.564	35.167	2	-6	4	35.202	35.907
-6	-4	3	5.178	4.365	-1	-11	3	4.618	5.355	-7	-13	4	13.069	10.933	4	-6	4	19.846	20.433
7	-5	3	9.438	10.940	-1	-11	3	7.597	7.143	-8	-12	4	19.367	13.923	6	-6	4	33.943	32.943
.5	-5	3	17.410	13.311	-3	-11	3	8.186	8.251	-5	-12	4	21.774	21.740	5	-5	4	15.183	17.417
4	0	0	112.826	115.366	-5	-11	3	11.563	13.330	-4	-12	4	17.543	15.767	4	0	0	112.826	115.366
3	-5	3	50.793	52.413	-7	-11	3	13.242	15.100	-2	-12	4	5.115	2.913	3	-5	4	56.254	55.709
1	-5	3	18.796	19.322	-8	-12	3	16.868	15.332	0	-12	4	44.484	43.520	1	-5	4	11.961	9.495
-1	-5	3	9.109	7.053	-6	-12	3	44.761	43.397	-2	-12	4	8.145	7.833	-1	-5	4	32.777	32.742
-3	-5	3	44.345	45.035	-4	-12	3	23.171	22.755	4	-12	4	9.144	10.920	-3	-5	4	22.767	22.553
-5	-5	3	30.918	31.441	-2	-12	3	9.161	3.001	5	-11	4	14.922	15.201	-7	-5	4	49.177	47.551
-7	-5	3	26.359	23.318	4	0	0	112.826	115.303	-3	-11	4	56.555	54.911	-9	-5	4	13.751	14.033
-9	-5	3	21.613	22.635	0	-12	3	25.954	27.970	-1	-11	4	46.089	47.039	-10	-4	4	31.172	35.003
-10	-6	3	8.243	8.575	2	-12	3	37.990	39.447	-3	-11	4	44.917	44.013	-8	-4	4	28.407	26.054
-8	-6	3	9.479	7.000	4	-12	3	25.001	25.371	-5	-11	4	4.202	1.937	-6	-4	4	4.006	2.953
-6	-6	3	15.297	18.671	5	-13	3	31.051	31.333	-7	-11	4	59.262	53.410	-4	-4	4	34.728	36.737
-4	-6	3	40.847	39.553	3	-13	3	18.328	17.000	-8	-10	4	13.901	12.492	-2	-4	4	17.687	17.073
-2	-6	3	9.028	10.023	1	-13	3	3.827	4.732	-5	-10	4	9.889	9.633	0	-4	4	37.753	39.275
0	-6	3	8.948	8.219	-1	-13	3	23.166	25.003	4	0	0	112.826	115.300	2	-4	4	8.383	9.471
2	-6	3	5.628	5.770	-3	-13	3	27.432	29.005	-4	-10	4	5.842	4.010	4	-4	4	29.267	28.064
-4	-6	3	8.682	8.032	-5	-13	3	24.055	23.700	-2	-10	4	33.203	31.157	6	-4	4	16.440	15.203
7	-7	3	19.234	19.552	-7	-13	3	8.497	9.540	4	-10	4	10.985	10.317	7	-3	4	39.837	39.755
5	-7	3	5.034	7.170	-6	-14	3	8.826	9.543	5	-9	4	13.479	11.003	5	-3	4	35.577	35.101
3	-7	3	43.601	42.501	-4	-14	3	1.963	3.211	3	-9	4	54.834	57.420	3	-3	4	5.299	5.123
1	-7	3	21.295	20.970	-2	-14	3	5.582	5.248	1	-9	4	12.821	13.523	1	-3	4	10.326	10.831
4	0	0	112.826	115.366	0	-14	3	5.138	4.300	-1	-9	4	64.007	56.252	4	0	0	112.826	115.366
-1	-7	3	32.032	32.059	-2	-14	3	11.874	13.314	-3	-9	4	70.686	72.303	-1	-3	4	37.124	33.440
-3	-7	3	39.185	35.923	4	-14	3	16.215	17.330	-5	-9	4	16.452	14.013	-3	-3	4	41.932	43.023
-5	-7	3	19.835	17.430	3	-15	3	12.059	11.007	-7	-9	4	45.858	47.333	-5	-3	4	88.916	87.016
-7	-7	3	23.183	20.823	1	-15	3	16.758	13.033	-9	-9	4	18.351	15.077	-7	-3	4	11.973	11.351
-9	-7	3	4.959	4.959	-1	-15	3	13.473	12.755	-10	-8	4	28.960	30.909	-9	-3	4	28.453	28.407
-8	-8	3	16.902	14.611	-3	-15	3	0.825	2.357	-8	-8	4	8.567	7.353	-11	-3	4	27.801	27.192
-6	-8	3	63.695	62.068	4	0	0	112.826	115.303	-6	-8	4	50.747	53.337	-10	-2	4	3.152	4.103
-4	-8	3	44.744	45.538	-5	-15	3	6.771	3.616	-4	-8	4	45.690	43.294	-8	-2	4	49.980	46.834
-2	-8	3	8.480	11.033	-4	-15	3	19.633	18.817	-2	-8	4	5.091	3.028	-6	-2	4	54.240	35.314
0	-8	3	61.790	55.819	-2	-16	3	12.723	12.312	0	-8	4	68.111	72.457	-4	-2	4	57.091	55.461
2	-8	3	56.249	55.543	0	-16	3	23.829	23.330	2	-8	4	23.610	23.071	-2	-2	4	62.119	55.017
4	-8	3	27.230	25.514	2	-16	3	13.727	12.531	4	0	0	112.826	115.300	0	-2	4	64.151	53.005
6	-8	3	9.600	8.332	-1	-17	3	11.782	8.631	-4	-8	4	30.335	29.532	-2	-2	4	46.245	43.456
5	-9	3	40.916	35.800	-4	-16	4	16.452	15.034	6	-8	4	37.130	37.014	4	-2	4	53.720	52.919

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
6	-2	4	23.560	24.073	0	4	4	14.732	13.532	3	11	4	14.824	14.793	-4	8	5	20.458	20.528
7	-1	4	17.762	17.613	2	4	4	5.323	1.519	4	0	0	112.826	112.500	-2	8	5	31.039	36.157
5	-1	4	27.559	21.333	4	4	4	55.933	50.591	1	11	4	6.327	6.042	0	8	5	25.625	26.195
3	-1	4	4.433	5.413	6	4	4	8.082	7.442	-1	11	4	28.101	23.109	2	8	5	20.406	20.526
1	-1	4	51.700	52.741	5	5	4	20.343	19.333	-3	11	4	5.490	4.019	4	8	5	24.291	24.264
4	0	0	112.826	113.500	3	5	4	15.257	15.333	-5	11	4	9.704	9.703	3	7	5	8.667	7.030
-3	-1	4	11.291	11.730	1	5	4	36.910	37.753	-7	11	4	20.181	19.134	4	0	0	112.826	112.500
-5	-1	4	44.553	46.330	-1	5	4	12.677	12.537	-8	12	4	24.037	23.130	1	7	5	33.452	33.057
-7	-1	4	3.169	1.470	-3	5	4	25.480	25.163	-6	12	4	8.636	9.110	-1	7	5	3.862	4.035
-9	-1	4	16.521	15.101	-5	5	4	6.102	6.543	-2	12	4	22.809	23.079	-7	5	27.513	26.329	
-11	-1	4	5.836	2.321	-7	5	4	23.021	22.640	0	12	4	15.384	14.571	-5	7	5	7.510	7.213
-10	0	4	10.056	9.704	-9	5	4	15.523	15.602	2	12	4	4.445	6.450	-7	7	5	17.676	13.770
-8	0	4	42.868	42.952	-10	6	4	31.259	32.130	-1	13	4	11.967	12.563	-9	7	5	24.459	24.930
-6	0	4	53.524	52.143	4	0	0	112.826	113.500	-1	13	4	24.234	24.250	-10	6	5	26.087	26.040
-4	0	4	6.592	6.381	-8	6	4	23.102	23.023	-3	13	4	20.504	21.172	-8	6	5	24.114	24.105
-2	0	4	157.079	154.733	-6	6	4	8.228	8.243	-7	13	4	9.658	9.233	-6	6	5	84.719	84.003
0	0	4	41.909	41.971	-4	6	4	43.878	43.027	-6	14	4	8.653	8.473	-4	6	5	25.423	25.446
2	0	4	64.446	55.187	-2	6	4	11.366	12.223	-4	14	4	28.563	29.332	-2	6	5	81.673	85.124
4	0	4	61.940	52.655	0	6	4	52.075	52.020	-2	14	4	17.947	18.240	0	6	5	44.340	44.933
6	0	4	12.047	11.800	2	6	4	52.681	53.154	0	14	4	9.577	9.144	2	6	5	10.420	10.334
7	1	4	22.583	23.393	6	6	4	38.700	37.449	4	0	0	112.826	113.500	4	6	5	45.340	45.571
5	1	4	26.439	27.142	5	7	4	18.190	18.312	-1	15	4	13.167	13.335	5	5	5	19.558	19.202
3	1	4	22.219	22.456	3	7	4	12.734	14.378	-3	15	4	6.275	6.343	3	5	5	35.646	35.006
1	1	4	66.022	50.732	1	7	4	8.746	9.570	-5	15	4	7.216	6.523	1	5	5	39.225	39.297
-1	1	4	34.526	33.155	-1	7	4	8.393	7.343	-4	14	5	37.412	37.663	-1	5	5	54.586	53.074
4	0	0	112.826	113.500	-3	7	4	11.020	11.505	-2	14	5	23.010	22.703	-3	5	5	82.520	83.052
-5	1	4	64.244	53.473	-5	7	4	6.789	6.114	1	13	5	11.286	13.447	-5	5	5	41.557	40.020
-7	1	4	19.846	19.846	-7	7	4	16.227	16.075	-1	13	5	21.699	21.334	-4	0	0	112.826	113.500
-9	1	4	33.383	33.592	-9	7	4	1.8C7	2.082	-3	13	5	37.095	36.214	-9	5	5	48.225	43.350
-11	1	4	1.126	3.232	-10	8	4	13.496	10.056	-5	13	5	16.002	15.209	-10	4	5	36.114	35.553
-10	2	4	23.016	24.500	-8	8	4	12.030	11.325	-6	12	5	23.408	23.711	-8	4	5	42.458	42.258
-8	2	4	11.355	5.213	-6	8	4	10.437	11.024	-4	12	5	25.688	24.080	-6	4	5	14.853	10.515
-6	2	4	2.500	2.930	-4	8	4	55.140	50.111	-2	12	5	31.369	31.737	-4	4	5	73.676	74.073
-4	2	4	61.577	59.934	-4	0	0	112.826	113.500	0	12	5	20.666	19.754	0	4	5	48.121	49.236
-2	2	4	53.773	53.557	-2	8	4	49.922	50.843	2	12	5	15.084	16.133	2	4	5	43.814	43.033
0	2	4	40.639	41.035	0	8	4	38.509	39.800	1	11	5	20.660	20.541	4	4	5	7.429	8.004
-2	2	4	14.276	14.431	-2	8	4	17.150	13.509	-1	11	5	12.423	12.300	5	3	5	29.412	29.335
4	2	4	14.923	11.630	4	8	4	0.306	0.282	-5	11	5	10.466	12.031	3	3	5	31.507	32.095
6	2	4	26.641	20.371	5	9	4	9.750	9.443	-7	11	5	15.113	13.747	1	3	5	20.753	21.737
5	3	4	4.439	5.323	-3	9	4	15.215	16.231	-4	0	0	112.826	115.360	-1	3	5	56.191	55.556
3	3	4	18.386	17.710	1	9	4	24.343	23.912	-6	10	5	24.216	23.338	-3	3	5	36.853	37.414
1	3	4	23.408	24.832	-1	9	4	45.125	40.123	-4	10	5	18.293	17.032	-5	3	5	51.273	51.730
-1	3	4	30.641	30.337	-3	9	4	27.455	21.151	-2	10	5	3.025	2.901	-7	3	5	27.645	23.234
-3	3	4	21.336	21.153	-5	9	4	12.850	11.694	0	10	5	19.182	19.451	-9	3	5	23.564	22.070
-7	3	4	12.625	13.309	-7	9	4	14.657	15.200	2	10	5	13.341	12.310	-11	3	5	16.723	15.255
-4	0	0	112.826	113.500	-9	9	4	28.898	29.241	3	9	5	47.313	46.125	-10	2	5	12.452	13.133
-9	3	4	7.285	0.455	-8	10	4	8.861	8.319	1	9	5	18.934	18.211	4	0	0	112.826	113.500
-11	3	4	14.567	14.733	-6	10	4	17.099	15.333	-3	9	5	75.622	70.677	-8	2	5	20.279	20.250
-10	4	4	27.178	27.354	-4	10	4	45.189	45.001	-5	9	5	6.298	3.771	-6	2	5	12.452	12.158
-8	4	4	40.305	41.719	-2	10	4	50.713	50.877	-7	9	5	7.724	7.915	-4	2	5	21.232	21.210
-6	4	4	28.159	29.140	0	10	4	11.014	10.220	-9	9	5	40.259	41.145	-2	2	5	30.341	31.230
-4	4	4	1.057	1.031	-2	10	4	5.640	5.173	-8	8	5	33.885	34.335	0	2	5	18.045	17.330
-2	4	4	65.358	50.105	4	10	4	20.363	20.678	-6	8	5	22.375	21.297	2	2	5	2.806	3.300

SUENO, PREWITT, AND PAPIKE - HIGH ALBITE - 24 DEG. C

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	
-4	2	5	27.339	27.172	4	-4	5	21.024	21.094	-6	-12	5	24.386	26.015	-1	-7	6	23.340	30.151	
5	1	5	53.553	51.439	4	0	0	112.826	115.350	-4	-12	5	16.937	17.039	-3	-7	6	61.421	65.711	
1	1	5	32.881	32.547	5	-5	5	6.841	5.617	-2	-12	5	29.671	32.006	-5	-7	6	36.789	38.201	
-1	1	5	84.315	87.521	3	-5	5	15.584	14.072	0	-12	5	4.318	5.638	-9	-7	6	24.349	26.476	
-3	1	5	44.143	40.137	1	-5	5	49.298	52.007	2	-12	5	7.516	8.022	-10	-6	6	1.449	1.135	
-5	1	5	55.902	59.179	-1	-5	5	1.443	3.705	1	-13	5	29.400	29.350	-8	-6	6	4.506	4.522	
-7	1	5	40.986	39.158	-3	-5	5	40.062	42.143	-1	-13	5	21.954	22.176	-6	-6	6	6.789	3.705	
-9	1	5	11.869	12.631	-5	-5	5	24.043	23.747	-3	-13	5	9.935	10.362	-4	-6	6	12.659	12.950	
-11	1	5	48.554	48.005	-7	-5	5	9.392	1.757	4	0	0	112.826	115.350	-2	-6	6	9.854	9.771	
-10	0	5	45.760	49.393	-9	-5	5	38.648	39.318	-5	-13	5	6.483	7.738	0	-6	6	22.456	21.032	
-8	0	5	31.744	32.322	-10	-6	5	25.833	25.259	-7	-13	5	24.817	24.313	2	-6	6	3.948	1.355	
-6	0	5	42.845	42.520	-8	-6	5	14.645	12.383	-6	-14	5	3.972	0.738	4	-6	6	11.389	9.999	
-4	0	5	108.341	109.752	-6	-6	5	24.447	26.493	-4	-14	5	6.800	7.610	3	-5	6	23.077	32.879	
4	0	0	112.826	115.300	-4	-6	5	57.813	55.633	-2	-14	5	3.723	5.613	1	-5	6	20.054	15.456	
-2	0	5	24.920	24.367	-2	-6	5	12.475	14.478	0	-14	5	12.013	12.692	4	0	0	112.826	115.300	
0	0	5	43.601	45.717	0	-6	5	23.933	24.370	-1	-15	5	22.161	22.031	-1	-5	6	3.637	4.639	
2	0	5	54.234	53.350	2	-6	5	22.051	21.367	-3	-15	5	1.911	3.512	-3	-5	6	26.133	24.040	
4	0	5	4.745	6.722	4	-6	5	9.952	11.321	-5	-15	5	10.599	9.377	-5	-5	6	6.056	6.038	
6	0	5	33.095	31.724	5	-7	5	8.243	4.203	-4	-14	6	18.383	13.773	-7	-5	6	18.420	17.332	
5	-1	5	15.569	14.220	3	-7	5	6.119	1.109	-2	-14	6	24.678	25.122	-9	-5	6	15.950	14.353	
1	-1	5	13.427	11.376	1	-7	5	18.732	15.308	-1	-13	6	37.609	35.322	-10	-4	6	14.288	13.317	
-1	-1	5	28.269	29.763	-1	-7	5	42.539	40.440	-5	-13	6	24.424	24.033	-8	-4	6	16.008	15.348	
-3	-1	5	4.837	1.579	4	0	0	112.826	115.366	-6	-12	6	27.541	25.311	-6	-4	6	35.005	35.130	
-5	-1	5	5.478	3.026	-3	-7	5	26.860	25.751	-2	-12	6	15.730	15.350	-4	-4	6	11.845	15.473	
-7	-1	5	20.527	13.933	-7	-7	5	21.047	22.157	0	-12	6	24.770	24.342	-2	-4	6	18.420	13.902	
-9	-1	5	9.721	10.344	-9	-7	5	16.350	14.919	1	-11	6	36.824	35.403	0	-4	6	38.561	37.040	
-11	-1	5	14.409	10.052	-8	-8	5	21.728	23.329	4	0	0	112.826	115.350	2	-4	6	13.358	11.398	
-10	-2	5	52.814	53.330	-6	-8	5	37.770	34.830	-1	-11	6	11.540	11.623	-4	-4	6	9.098	3.344	
-8	-2	5	36.408	35.746	-4	-8	5	34.416	31.470	-3	-11	6	70.241	53.329	3	-3	6	24.857	23.931	
-6	-2	5	28.794	27.930	-2	-8	5	51.579	50.317	-5	-11	6	8.255	9.117	1	-3	6	27.507	28.434	
-4	-2	5	71.483	72.300	0	-8	5	10.905	11.030	-7	-11	6	31.998	32.110	-1	-3	6	63.539	63.105	
-2	-2	5	7.579	5.933	2	-8	5	10.731	10.443	-8	-10	6	18.236	13.429	-3	-3	6	45.055	43.395	
0	-2	5	51.671	51.170	4	-8	5	27.876	23.073	-6	-10	6	12.059	10.329	-5	-3	6	64.157	50.053	
4	0	0	112.825	115.360	3	-9	5	8.919	1.114	-4	-10	6	21.526	22.153	-7	-3	6	4.653	2.273	
2	-2	5	31.565	33.050	1	-9	5	25.365	22.927	-2	-10	6	33.210	32.333	-9	-3	6	27.761	20.350	
4	-2	5	3.192	3.014	-1	-9	5	32.610	33.645	0	-10	6	7.308	5.339	4	0	0	112.826	115.350	
6	-2	5	8.405	8.667	-3	-9	5	33.781	32.533	-2	-10	6	15.349	15.116	-8	-2	6	26.375	23.710	
5	-3	5	40.813	40.132	-5	-9	5	32.211	31.378	3	-9	6	30.324	29.331	-6	-2	6	16.735	13.320	
3	-3	5	14.224	14.003	-9	-9	5	34.549	33.251	1	-9	6	27.022	27.116	-4	-2	6	17.664	15.920	
1	-3	5	5.969	6.014	-8	-10	5	1.345	2.308	-1	-9	6	16.753	14.335	-2	-2	6	23.539	22.333	
-1	-3	5	84.725	88.729	-6	-10	5	2.142	0.815	-3	-9	6	52.081	54.505	0	-2	6	21.001	22.107	
-3	-3	5	1.749	2.015	4	0	0	112.826	115.356	-5	-9	6	19.673	17.071	2	-2	6	30.889	29.571	
-5	-3	5	79.645	93.333	-2	-10	5	10.241	1.309	-7	-9	6	8.642	11.820	4	-2	6	23.766	23.354	
-7	-3	5	55.591	57.095	0	-10	5	9.502	10.782	-9	-9	6	20.175	18.031	3	-1	6	9.363	3.533	
-9	-3	5	5.392	3.373	2	-10	5	9.704	9.213	-8	-8	6	9.000	3.335	1	-1	6	14.120	14.103	
-11	-3	5	44.380	45.073	-4	-10	5	6.812	3.702	-6	-8	6	48.646	50.217	-1	-1	6	13.179	13.822	
-10	-4	5	21.468	19.930	3	-11	5	16.186	19.039	-4	-8	6	7.389	7.148	-5	-1	6	20.089	18.930	
-8	-4	5	7.868	5.752	1	-11	5	19.044	20.203	4	0	0	112.826	115.350	-7	-1	6	10.887	10.039	
-6	-4	5	34.832	33.236	-1	-11	5	14.743	15.263	-2	-8	6	24.182	23.118	-9	-1	6	10.506	3.839	
-4	-4	5	45.673	47.153	-3	-11	5	10.062	11.076	0	-8	6	47.313	48.214	-11	-1	6	3.660	1.705	
-2	-4	5	35.854	33.780	-5	-11	5	8.930	9.732	2	-8	6	11.852	11.278	-10	0	6	11.205	12.053	
0	-4	5	28.061	28.678	-7	-11	5	7.476	1.134	3	-7	6	23.547	22.410	-8	0	6	20.568	20.478	
1	2	-4	5	41.251	42.512	-8	-12	5	15.667	13.300	1	-7	6	8.844	0.620	-6	0	6	12.555	14.210

SUENO, PREWITT, AND PAPKE - HIGH ALBITE - 24 DEG. C

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-4	0	6	18.155	17.754	-3	7	6	8.844	7.753	-4	6	7	29.977	30.520	-8	-2	7	9.531	9.431
4	0	0	112.826	115.306	-5	7	6	10.749	11.232	-2	6	7	70.651	70.030	4	0	0	112.826	115.300
-2	0	6	41.113	40.137	-7	7	6	2.090	1.132	0	6	7	15.032	14.504	-6	-2	7	31.334	31.033
0	0	6	2.933	3.112	-8	8	6	14.841	14.303	2	6	7	28.678	27.213	-4	-2	7	40.259	31.453
2	0	6	31.975	31.543	-6	8	6	16.920	16.511	1	5	7	56.185	59.060	-2	-2	7	6.309	5.539
4	0	6	10.853	10.769	-4	8	6	10.587	11.002	-1	5	7	13.185	12.640	0	-2	7	40.883	41.033
-3	1	6	33.181	33.557	-2	8	6	11.164	11.277	-3	5	7	22.357	22.870	-2	-2	7	18.859	17.836
1	1	6	4.751	4.373	4	0	0	112.826	115.300	-5	5	7	41.540	41.092	3	-3	7	39.652	39.320
-1	1	6	21.353	21.308	0	8	6	24.049	24.004	-7	5	7	26.797	27.930	1	-3	7	15.452	15.459
-3	1	6	65.583	65.934	2	8	6	3.700	2.455	-9	5	7	48.623	49.182	-1	-3	7	33.637	32.037
-5	1	6	45.136	45.055	1	9	6	16.735	15.691	-10	4	7	32.217	32.322	-3	-3	7	42.487	42.932
-7	1	6	16.135	15.140	-1	9	6	8.139	7.733	-8	4	7	15.794	14.784	-7	-3	7	61.138	62.936
-9	1	6	22.427	23.974	-3	9	6	22.669	23.670	-6	4	7	25.983	26.114	-9	-3	7	9.555	8.521
-11	1	6	19.055	20.314	-5	9	6	43.058	43.083	-4	4	7	31.478	31.049	-10	-4	7	12.163	12.543
-10	2	6	20.603	19.722	-7	9	6	10.385	11.574	4	0	0	112.826	115.300	-8	-4	7	29.215	30.231
-3	2	6	16.896	16.329	-9	9	6	12.642	12.953	0	4	7	27.730	30.950	-6	-4	7	11.193	13.372
-6	2	6	26.346	23.710	-8	10	6	29.008	29.033	2	4	7	12.244	11.780	-4	-4	7	5.929	4.817
-4	2	6	5.224	5.150	-6	10	6	18.247	18.011	3	3	7	19.904	20.043	-2	-4	7	30.445	31.373
-2	2	6	19.275	18.543	-2	10	6	32.315	32.639	1	3	7	27.865	29.000	0	-4	7	20.123	22.022
0	2	6	20.908	21.042	0	10	6	19.587	21.339	-1	3	7	21.619	21.010	2	-4	7	3.440	4.751
2	2	6	2.898	2.472	-1	11	6	5.946	7.110	-3	3	7	39.133	38.800	4	0	0	112.826	115.300
4	2	6	13.543	12.110	-3	11	6	25.371	25.367	-5	3	7	38.890	39.417	1	-5	7	37.986	37.333
4	0	0	112.826	115.300	-5	11	6	21.734	22.223	-7	3	7	20.083	20.674	-1	-5	7	24.205	23.572
-3	3	6	5.882	4.653	-7	11	6	19.182	20.554	-9	3	7	25.584	25.503	-3	-5	7	23.154	21.039
-1	3	6	6.136	5.956	-6	12	6	4.832	5.354	-10	2	7	10.397	10.337	-5	-5	7	33.770	33.234
-1	3	6	2.886	2.700	-4	12	6	10.887	10.650	-8	2	7	29.868	20.156	-7	-5	7	15.575	13.772
-3	3	6	12.856	12.549	4	0	0	112.826	115.300	-4	2	7	8.532	8.050	-9	-5	7	26.773	23.491
-5	3	6	21.012	19.733	0	12	6	6.627	6.036	-2	2	7	34.740	35.271	-6	-6	7	20.204	20.513
-9	3	6	7.663	6.637	-3	13	6	5.392	4.710	0	2	7	1.720	3.219	-4	-6	7	34.939	35.031
-10	4	6	15.956	16.260	-5	13	6	8.451	10.232	2	2	7	13.242	12.030	-2	-6	7	4.139	4.529
-8	4	6	13.456	12.930	-3	11	7	4.243	1.920	3	1	7	38.988	37.500	0	-6	7	21.555	18.510
-6	4	6	6.662	4.990	-5	11	7	3.903	4.824	1	1	7	15.667	15.241	2	-6	7	16.158	17.153
-2	4	6	14.576	15.314	-6	10	7	6.293	7.034	-1	1	7	49.702	49.430	1	-7	7	29.613	23.413
0	4	6	19.506	9.979	-4	10	7	4.116	5.075	4	0	0	112.826	115.300	-1	-7	7	6.727	5.233
2	4	6	14.668	14.337	-2	10	7	17.514	16.201	-3	1	7	11.505	11.333	-3	-7	7	13.508	11.273
4	4	6	18.034	17.141	-1	9	7	9.109	9.035	-5	1	7	17.526	17.333	-5	-7	7	49.212	47.513
-3	5	6	42.700	42.273	-3	9	7	42.377	42.279	-7	1	7	50.1C1	50.034	-7	-7	7	10.951	11.053
1	5	6	19.148	19.232	-5	9	7	37.765	33.503	-9	1	7	7.932	8.552	-9	-7	7	12.082	9.034
-1	5	6	9.392	10.078	-7	9	7	8.295	8.020	-10	0	7	36.287	36.743	-8	-8	7	42.683	41.053
-3	5	6	33.660	34.502	-8	8	7	28.922	28.892	-8	0	7	9.282	11.243	-6	-8	7	15.208	13.031
-5	5	6	22.069	23.133	-6	8	7	14.876	13.630	-6	0	7	42.423	41.002	4	0	0	112.826	115.300
4	0	0	112.826	115.300	-4	8	7	28.338	28.315	-4	0	7	53.524	54.080	-4	-8	7	9.681	10.110
-7	5	6	16.054	16.930	-2	8	7	22.317	23.303	-2	0	7	10.801	9.573	-2	-8	7	54.811	53.177
-9	5	6	16.054	16.276	0	8	7	25.861	25.820	0	0	7	39.312	33.020	0	-8	7	7.314	7.334
-10	6	6	11.343	9.233	1	7	7	23.610	24.432	2	0	7	22.069	21.434	2	-8	7	22.311	21.713
-8	6	6	31.715	31.310	-1	7	7	2.598	1.732	3	-1	7	10.339	9.861	-1	-9	7	16.504	15.511
-6	6	6	13.468	12.033	4	0	0	112.826	115.300	1	-1	7	1.563	2.409	-1	-9	7	5.773	2.003
-4	6	6	12.527	11.675	-3	7	7	4.520	4.912	-1	-1	7	12.024	12.150	-3	-9	7	2.101	3.053
-2	6	5	3.423	3.299	-5	7	7	.20.464	20.301	-3	-1	7	9.167	10.630	-5	-9	7	35.357	34.973
0	6	6	39.196	39.713	-7	7	7	12.659	12.244	-5	-1	7	3.319	2.942	-7	-9	7	1.310	4.150
2	6	6	7.055	7.240	-9	7	7	26.757	26.597	-7	-1	7	6.991	7.016	-8	-10	7	15.274	14.534
-3	7	6	13.317	9.375	-8	6	7	47.590	43.035	-9	-1	7	14.738	14.555	-6	-10	7	20.262	20.433
1	7	6	16.706	15.815	-6	6	7	46.833	46.024	-10	-2	7	46.383	47.015	-4	-10	7	6.188	5.053

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	-10	7	10.189	10.635	-6	-2	8	6.154	4.451	-5	9	8	24.459	22.630
0	-10	7	8.734	7.142	-4	-2	8	16.689	15.044	-3	5	9	17.970	17.174
-1	-11	.	24.020	23.533	-2	-2	8	10.391	10.271	-5	5	9	24.251	23.318
-3	-11	7	4.012	3.390	0	-2	8	12.388	11.503	-6	4	9	28.927	23.322
-5	-11	7	43.959	44.038	1	-1	8	10.916	11.142	4	0	0	112.826	115.306
-7	-11	7	7.037	5.116	-1	-1	8	4.676	0.125	-4	4	9	21.815	20.385
-6	-12	7	3.417	3.997	-3	-1	8	8.572	6.474	-2	4	9	18.190	13.117
-4	-12	7	3.723	4.437	-5	-1	8	7.770	0.117	-3	3	9	16.233	14.032
4	0	0	112.826	115.303	-9	-1	8	14.564	13.331	-5	3	9	33.891	33.155
-2	-12	7	26.739	26.537	-8	0	8	4.583	1.310	-7	3	9	16.896	17.231
-3	-13	7	17.168	17.114	-6	0	8	12.839	14.221	-8	2	9	15.944	15.919
-3	-11	8	22.236	22.237	-4	0	8	17.052	17.718	-6	2	9	25.763	24.483
-6	-10	8	6.258	2.513	-2	0	8	6.442	6.353	-4	2	9	6.113	4.927
-4	-10	8	5.519	4.910	0	0	8	2.026	2.935	-2	2	9	17.104	17.619
-2	-10	8	9.923	8.152	1	1	8	28.817	29.244	-1	1	9	8.647	8.339
-1	-9	8	12.654	10.339	-1	1	8	39.162	33.739	-3	1	9	47.353	45.346
-3	-9	8	23.564	23.000	-3	1	8	35.392	35.868	-7	1	9	22.698	22.332
-5	-9	8	25.977	26.310	4	0	0	112.826	115.303	-8	0	9	12.001	11.730
-7	-9	8	5.571	4.443	-5	1	8	11.459	11.124	-6	0	9	40.374	38.457
-8	-8	8	8.671	3.413	-7	1	8	33.216	34.472	-4	0	9	28.378	29.342
-6	-8	8	20.712	21.199	-9	1	8	37.736	33.120	-2	0	9	16.562	16.120
-4	-8	8	12.457	14.316	-8	2	8	15.251	15.079	-1	-1	9	4.976	3.111
-2	-8	8	20.043	21.039	-6	2	8	10.737	10.446	4	0	0	112.826	115.300
0	-8	8	14.992	13.517	-4	2	8	22.242	20.944	-7	-1	9	5.559	2.281
-1	-7	8	36.102	35.914	-2	2	8	14.841	12.712					
-3	-7	8	15.228	14.904	0	2	8	2.401	0.214					
-5	-7	8	9.611	3.679	1	3	8	4.786	2.936					
-7	-7	8	37.245	37.714	-1	3	8	15.038	14.534					
-3	-6	8	5.992	3.220	-3	3	8	4.774	3.835					
4	0	0	112.826	115.303	-5	3	8	9.548	9.032					
-6	-6	8	5.530	2.317	-7	3	8	27.657	21.317					
-4	-6	8	12.746	13.423	-9	3	8	3.290	0.238					
-2	-6	8	8.769	7.256	-8	4	8	3.966	2.332					
0	-6	8	7.545	3.722	-6	4	8	4.682	2.993					
1	-5	8	18.680	17.824	-4	4	8	4.093	2.018					
-1	-5	8	9.513	7.547	-2	4	8	6.702	7.436					
-3	-5	8	6.460	0.151	-1	5	8	43.659	43.350					
-5	-5	8	9.456	9.010	4	0	0	112.826	115.300					
-7	-5	8	10.743	10.310	-3	5	8	13.716	13.532					
-9	-5	8	5.605	4.233	-5	5	8	4.532	5.059					
-8	-4	8	4.624	1.917	-7	5	8	28.101	29.029					
-6	-4	8	21.232	19.453	-8	6	8	32.921	32.920					
-4	-4	8	9.063	6.999	-4	6	8	15.725	15.923					
-2	-4	8	21.365	19.512	-2	6	8	11.118	9.315					
0	-4	8	6.771	9.133	0	6	8	16.469	15.011					
1	-3	8	17.780	16.512	-1	7	8	21.468	20.793					
-1	-3	8	61.865	50.720	-3	7	8	7.377	2.033					
-3	-3	8	8.070	5.314	-5	7	8	10.506	10.619					
-5	-3	8	2.286	4.373	-7	7	0	14.310	13.507					
-7	-3	8	42.954	41.807	-6	8	0	1.645	1.142					
4	0	0	112.826	115.306	-4	8	8	14.079	13.038					
-9	-3	8	37.060	35.599	-2	8	8	11.620	11.150					
-8	-2	8	13.727	13.702	-3	9	8	2.546	1.817					

ATOM	PARAMETER	OLD	CHANGE	NEW	ERRCK	SHIFT/ERROR
	EXTINCTION CORRECTION	0.0		0.0		
	SCALE FACTOR 1	1.7323	0.0000	1.7323	0.00393	0.00
ATOM 1	NAI	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.2736595	0.000002	0.2736597	0.0002879	0.00
	Y	0.0372630	-0.000002	0.0372631	0.0002955	0.00
	Z	0.1329437	-0.000000	0.1329436	0.0005049	-0.00
	BETA11	0.0053464	0.000003	0.0053467	C.0003451	0.00
	BETA22	0.0177929	-0.000005	0.0177924	0.0003635	-0.00
	BETA33	0.0434692	-0.000009	0.0434683	0.0010063	-0.00
	BETA12	0.0317125	-0.000002	0.0317122	C.0002658	-0.00
	BETA13	0.0310725	C.000004	0.0310732	C.0004638	0.00
	BETA23	-0.0210421	0.000007	-0.0210414	0.0005168	0.00
ATOM 2	TiO	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		C.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.0050264	0.000000	0.0090264	0.0001170	0.00
	Y	0.1347609	-0.000000	0.1649609	C.0006672	-0.00
	Z	0.2147673	-0.000001	0.2147673	0.0001367	0.00
	BETA11	0.0036697	0.000000	0.0036697	C.0001387	0.00
	BETA22	0.0012669	0.000000	0.0012669	C.0000462	C.CC
	BETA33	0.00149325	C.000000	0.0048325	C.0001823	0.00
	BETA12	-0.00102723	-0.000000	-0.0002724	C.0000662	-0.00
	BETA13	0.0021340	0.000000	0.0021341	0.0001315	0.00
	BETA23	0.0000682	0.000000	0.0000682	C.0000709	0.00
ATOM 3	TIM	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		C.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.0346371	-0.000001	0.0048369	0.0001164	0.00
	Y	0.8145427	-0.000000	0.8145427	C.0000673	-0.00
	Z	0.2290092	-0.000000	0.2290091	0.0001356	-0.00
	BETA11	0.0035484	-0.000000	0.0036483	0.0001399	-0.00
	BETA22	0.0012868	-0.000000	0.0012868	C.0000461	-0.00
	BETA33	0.0034522	0.000000	0.0046422	0.0001861	0.00
	BETA12	0.00105163	0.000001	0.0005164	C.0000665	0.00
	BETA13	0.00319468	-0.000000	0.0019468	0.0001320	-0.00
	BETA23	0.0002797	0.000000	0.0002797	C.0000710	0.00
ATOM 4	T2C	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		C.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.5702024	C.0000000	0.6902024	C.0001167	0.00
	Y	0.1371442	0.000000	0.1079442	0.0000676	0.00
	Z	0.3201655	-0.000000	0.3201654	C.0001358	-0.00
	BETA11	0.0032626	-0.000000	0.0032626	0.0001373	-0.00
	BETA22	0.0011642	0.000000	0.0011642	C.0000454	0.00
	BETA33	0.0057066	-0.000000	0.0057066	C.0001934	-0.00
	BETA12	0.0000291	-0.000000	C.0000291	C.0000592	-0.00
	BETA13	0.0016470	-0.000000	0.0016470	C.0001326	-0.00
	BETA23	0.0001623	-0.000000	0.0001623	0.0000711	-0.00

ATOM 5	T2M	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 2	0.75000		0.75000	
		OCCUPANCY SPECIES 4	0.25000		0.25000	
		TOTAL OCCUPANCY (FIXED) =	1.00000			
		X	0.6848633	0.0000000	0.6848633	0.0001166
		Y	0.8775541	0.0000000	0.8775541	0.CCCC667
		Z	0.3535050	0.0000000	0.3535050	C.0001384
		BETA11	0.0034787	0.0000000	0.0034787	C.0001383
		BETA22	0.0010380	-0.0000000	0.0010380	C.CCCC444
		BETA33	0.0057871	-0.0000000	0.0057871	0.0001937
		BETA12	0.0001688	-0.0000000	0.0001688	C.CCCC554
		BETA13	0.0019029	-0.0000000	0.0019029	C.0001330
		BETA23	0.0001830	-0.0000000	0.0001830	0.00007C6
ATOM 6	OA1	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 3	1.00000		1.00000	
		X	0.0054563	0.0000001	0.0054564	0.0003671
		Y	0.1350E65	-0.0000000	0.1350E65	C.0002015
		Z	0.9344556	-0.0000001	0.9844555	0.0004065
		BETA11	0.0058426	-0.0000000	0.0058426	0.0004861
		BETA22	0.0023891	-0.0000000	0.0023891	C.0001473
		BETA33	0.0085834	-0.0000001	0.0089834	C.0005876
		BETA12	0.0004135	0.0000000	0.0004135	C.CCC2C59
		BETA13	0.0054804	-0.0000000	0.0054804	0.0004468
		BETA23	0.0003176	-0.0000001	0.0003175	0.0002295
ATOM 7	OA2	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 3	1.00000		1.00000	
		X	0.5915697	0.0000001	0.5915697	C.0003147
		Y	0.9906965	0.0000001	0.9906966	C.0001861
		Z	0.2762850	-0.0000002	0.2762848	C.0003947
		BETA11	0.0045421	-0.0000000	0.0045421	C.0003899
		BETA22	0.0017708	-0.0000000	0.0017708	C.0001292
		BETA33	0.0103426	-0.0000001	0.0103426	0.0005850
		BETA12	-0.0001076	-0.0000000	-0.0001076	C.0001749
		BETA13	0.0023479	-0.0000001	0.0023479	C.0003920
		BETA23	0.00007C85	-0.0000000	C.0007085	0.0002158
ATOM 8	OBC	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 3	1.00000		1.00000	
		X	0.8211860	-0.0000002	0.8211861	C.0003508
		Y	0.1083959	-0.0000000	0.1083958	0.0002057
		Z	0.1990344	-0.0000001	0.1990343	0.0004258
		BETA11	0.0070561	-0.0000001	C.0070562	C.0004403
		BETA22	0.0026160	-0.0000001	0.0026159	0.00014E5
		BETA33	0.0125027	-0.0000000	0.0125026	C.0006429
		BETA12	-0.0003749	0.0000001	-0.0003748	C.0002000
		BETA13	0.0051263	-0.0000001	0.0057262	C.0004495
		BETA23	-0.0001687	-0.0000000	-0.0001687	C.0002421
ATOM 9	OBM	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 3	1.00000		1.00000	
		X	0.2183903	-0.0000000	0.2183903	C.0003590
		Y	0.8469657	-0.0000001	0.8469656	0.0002207
		Z	0.2454909	-0.0000001	0.2454907	0.0004486
		BETA11	0.0063970	-0.0000001	0.0068969	C.0004515
		BETA22	0.0033362	0.0000001	0.0033363	0.0001658
		BETA33	0.0142672	-0.0000002	0.0142670	C.0006542
		BETA12	0.0011242	-0.0000000	0.0011242	C.0002130
		BETA13	0.0061725	-0.0000002	0.0061723	C.0004728
		BETA23	-0.0001358	-0.0000000	-0.0001358	C.00026E4

ATOM 10 OGM EQUIPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 3 1.00000 1.00000
 X 0.3162232 -0.0000001 0.0162231 C.00C2320 -0.00
 Y 0.2901692 0.0000001 0.2901692 0.0001893 0.00
 Z 0.2770357 0.0000001 0.2770358 C.CC4CE5 0.00
 BETA11 0.0355117 -0.0000001 0.0059116 0.0004098 -0.00
 BETA22 0.0118290 0.0000001 0.0018291 C.0001333 0.00
 BETA33 0.0111260 -0.0000001 0.0111259 C.0006041 -0.00
 BETA12 -0.0005478 -0.0000000 -0.0005478 C.0001819 -0.00
 BETA13 0.0023144 -0.0000001 0.0033144 C.00C4134 -0.00
 BETA23 -0.0001412 0.0000000 -0.0001412 C.00C2229 0.00

ATOM 11 OGM EQUIPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 3 1.00000 1.00000
 X 0.0212921 -0.0000001 0.0212920 0.0003335 -0.00
 Y 0.6872633 -0.0000000 0.6872633 0.0001923 -0.00
 Z 0.2177698 0.0000001 0.2177698 C.CC3970 0.00
 BETA11 0.0366496 -0.0000001 0.0060495 0.0004155 -0.00
 BETA22 0.0019675 0.0000000 0.0019676 C.00C1351 0.00
 BETA33 0.0092195 -0.0000000 0.0092195 C.00C58C8 -0.00
 BETA12 0.0001362 0.0000001 0.0007362 0.0001848 0.00
 BETA13 0.0011909 -0.0000001 0.0014907 C.00C4CE4 -0.00
 BETA23 0.0001506 -0.0000001 0.0001505 C.0002204 -0.00

ATOM 12 OOO EQUIPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 3 1.00000 1.00000
 X 0.1358649 0.0000001 0.1958650 0.0003350 0.00
 Y 0.1122861 0.0000000 0.1122861 C.00C1946 0.00
 Z 0.3575861 -0.0000000 0.3875861 C.CC39C5 0.00
 BETA11 0.0361783 -0.0000000 0.0061783 0.0004139 -0.00
 BETA22 0.0122474 -0.0000000 0.022474 C.00C1402 -0.00
 BETA33 0.003d2285 -0.0000001 0.0082285 0.0005595 0.00
 BETA12 0.000CE636 0.0000000 0.0008636 0.0001875 0.00
 BETA13 0.00021016 -0.0000000 0.0021015 C.00C3979 -0.00
 BETA23 0.000C7751 -0.0000001 0.0007752 C.00C2208 0.00

ATOM 13 COM EQUIPOINT FRACTION = 1.000
 OCCUPANCY SPECIES 3 1.00000 1.00000
 X 0.1884823 0.0000001 0.1884823 0.0003440 0.00
 Y 0.3574983 0.0000000 0.674983 C.CC2C21 0.00
 Z 0.4265919 -0.0000001 0.4265919 0.0004035 -0.00
 BETA11 0.0064462 -0.0000001 0.0064461 0.00C4258 -0.00
 BETA22 0.0124242 0.0000001 0.024242 C.0001448 0.00
 BETA33 0.00EE852 -0.0000001 0.0086853 C.CC5784 0.00
 BETA12 0.0000346 0.0000001 0.0000347 C.00C1944 0.00
 BETA13 0.0012227 -0.0000001 0.0012226 C.00C4CE8 -0.00
 BETA23 -0.00017646 0.0000001 -0.00017645 0.0002275 0.00

MAXIMUM SHIFT/ERROR = -0.00

AVERAGE SHIFT/ERROR = 0.00

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	1	3	37.736	37.693	-4	-4	3	26.985	27.304	-6	-10	3	6.684	8.301	0	6	0	94.420	93.236
1	1	3	92.925	91.738	0	6	0	94.675	93.236	-4	-10	3	3.601	5.994	-6	-14	4	14.285	15.497
-1	1	3	44.777	40.175	-2	-4	3	22.677	21.000	-2	-10	3	11.344	11.163	-4	-14	4	6.598	4.864
-3	1	3	51.059	48.108	0	-4	3	58.937	59.258	0	-10	3	18.464	16.545	-2	-14	4	31.363	31.555
-5	1	3	50.353	49.399	2	-4	3	88.201	88.800	2	-10	3	3.759	1.813	0	-14	4	7.394	4.182
-7	1	3	17.477	18.803	4	-4	3	38.975	39.589	4	-10	3	7.386	4.650	2	-14	4	25.329	25.596
-9	1	3	5.655	4.666	6	-4	3	2.918 *	3.699	6	-10	3	3.631 *	1.762	3	-13	4	21.153	20.344
-11	1	3	27.236	27.424	7	-5	3	10.297	11.234	5	-11	3	11.318	12.096	1	-13	4	23.770	24.387
-10	0	3	14.018	13.429	5	-5	3	14.946	16.214	3	-11	3	9.103	8.796	-1	-13	4	6.309	6.046
-8	0	3	54.405	53.326	3	-5	3	47.743	49.090	1	-11	3	3.766	2.411	-3	-13	4	3.984 *	4.389
-6	0	3	6.966	8.261	1	-5	3	19.151	16.712	-1	-11	3	9.564	10.712	-5	-13	4	30.860	29.816
-4	0	3	112.970	109.315	-1	-5	3	2.013	8.411	0	6	0	94.412	93.236	-7	-13	4	12.400	12.322
-0	6	0	94.521	93.236	-3	-5	3	46.046	46.815	-3	-11	3	14.578	11.343	-8	-12	4	13.898	13.585
-2	0	3	14.375	18.207	-5	-5	3	32.831	23.612	-5	-11	3	9.238	10.036	-6	-12	4	11.540	12.439
0	0	3	32.403	31.162	-7	-5	3	29.745	26.671	-7	-11	3	16.951	17.396	-4	-12	4	20.079	19.819
2	0	3	49.655	49.442	-9	-5	3	19.129	19.484	-8	-12	3	15.715	15.895	-2	-12	4	9.685	6.261
4	0	3	21.780	22.999	-10	-6	3	8.164	9.707	-6	-12	3	37.435	37.599	0	-12	4	38.937	39.300
6	0	3	7.022	7.383	-8	-6	3	9.016	6.875	-4	-12	3	16.151	15.416	2	-12	4	5.884	5.796
8	0	3	21.821	21.398	-6	-6	3	5.231	4.729	-2	-12	3	3.875	7.409	4	-12	4	7.266	7.598
7	-1	3	7.063	6.620	-4	-6	3	39.808	38.061	0	-12	3	24.446	26.778	5	-11	4	13.072	12.976
5	-1	3	13.766	13.417	-2	-6	3	2.227	6.501	2	-12	3	32.505	34.228	3	-11	4	45.422	45.340
3	-1	3	26.405	26.759	0	-6	3	5.445	0.819	4	-12	3	22.820	22.973	0	6	0	94.543	93.236
1	-1	3	55.715	53.041	0	6	0	94.454	93.236	5	-13	3	25.869	25.775	1	-11	4	5.745	4.740
-1	-1	3	19.542	17.180	2	-6	3	4.536	6.002	3	-13	3	15.171	14.908	-1	-11	4	36.913	36.041
-3	-1	3	20.710	19.966	4	-6	3	5.148	3.212	1	-13	3	2.828	3.195	-3	-11	4	37.101	37.223
-5	-1	3	22.625	22.098	6	-6	3	4.183	3.949	-1	-13	3	23.094	22.369	-5	-11	4	3.522 *	3.617
-7	-1	3	6.596	5.824	7	-7	3	14.656	13.500	-3	-13	3	25.066	27.272	-7	-11	4	45.708	44.798
-9	-1	3	5.772	5.945	5	-7	3	4.701	4.474	-5	-13	3	25.768	26.248	-9	-10	4	12.383	12.529
-11	-1	3	15.479	15.955	3	-7	3	39.574	37.719	-7	-13	3	3.380	0.564	-6	-10	4	8.303	7.356
-10	-2	3	20.499	20.194	1	-7	3	21.885	21.664	-6	-14	3	6.035	6.596	-4	-10	4	8.701	5.375
-8	-2	3	38.412	38.371	-1	-7	3	28.866	29.076	-4	-14	3	3.980 *	2.002	-2	-10	4	37.187	39.489
-6	-2	3	12.512	10.411	-3	-7	3	37.048	33.688	-2	-14	3	3.928 *	4.344	0	-10	4	5.589	0.834
-4	-2	3	34.442	35.032	-5	-7	3	22.197	21.363	0	6	0	94.499	93.236	2	-10	4	6.346	7.077
0	6	0	94.660	93.236	-7	-7	3	18.464	16.525	0	-14	3	3.395	4.692	4	-10	4	8.171	8.578
-2	-2	3	4.652	4.045	-9	-7	3	4.386	5.815	2	-14	3	14.536	14.262	5	-9	4	9.594	8.793
0	-2	3	4.236	1.584	-8	-8	3	11.517	9.656	4	-14	3	11.938	12.558	3	-9	4	48.273	49.016
2	-2	3	38.603	38.223	-6	-8	3	59.069	56.968	3	-15	3	7.694	5.828	1	-9	4	10.807	6.599
4	-2	3	18.956	19.439	-4	-8	3	34.728	33.643	1	-15	3	12.253	14.293	-1	-9	4	60.330	61.546
6	-2	3	1.540 *	1.601	-2	-8	3	11.498	11.478	-1	-15	3	9.410	5.764	-3	-9	4	60.928	61.177
8	-2	3	6.834	7.420	0	-8	3	60.616	59.281	-3	-15	3	4.104 *	2.863	-5	-9	4	9.775	6.626
7	-3	3	4.656	3.300	2	-8	3	48.445	45.736	-5	-15	3	4.758	2.162	-7	-9	4	39.234	40.572
5	-3	3	26.891	27.047	4	-8	3	25.498	24.384	-4	-16	3	15.197	15.379	-9	-9	4	11.697	8.195
3	-3	3	37.420	39.095	6	-8	3	6.568	7.144	-2	-16	3	8.535	7.400	0	6	0	94.401	93.236
1	-3	3	43.939	42.910	0	6	0	94.709	93.236	0	-16	3	20.225	20.569	-10	-8	4	34.397	34.325
-1	-3	3	15.238	11.863	5	-9	3	31.371	30.060	2	-16	3	12.527	11.273	-8	-8	4	8.153	7.679
-3	-3	3	18.719	18.985	3	-9	3	15.355	13.562	-1	-17	3	12.186	11.280	-6	-8	4	41.048	40.449
-5	-3	3	91.787	89.947	1	-9	3	22.475	22.471	-4	-16	4	11.712	10.207	-4	-8	4	51.540	53.371
-7	-3	3	25.100	25.073	-1	-9	3	28.592	26.504	-2	-16	4	26.620	27.365	-2	-8	4	3.229 *	2.375
-9	-3	3	12.219	11.197	-3	-9	3	50.338	49.279	0	-16	4	6.673	4.672	0	-8	4	67.668	70.082
-11	-3	3	24.007	24.009	-5	-9	3	14.407	12.500	1	-15	4	4.818	0.748	2	-8	4	23.890	22.287
-10	-4	3	8.224	8.848	-7	-9	3	19.287	16.420	-1	-15	4	22.437	22.348	4	-8	4	25.452	26.187
-8	-4	3	30.225	30.728	-9	-9	3	17.927	18.061	-3	-15	4	22.077	22.455	6	-8	4	32.080	32.825
-6	-4	3	65.276	66.064	-8	-10	3	7.101	5.178	-5	-15	4	5.659	0.834	5	-7	4	17.390	18.204

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
3	-7	4	10.229	13.183	4	-2	4	44.713	43.774	-6	4	4	29.602	30.289	-4	10	4	33.639	33.377
1	-7	4	59.290	61.252	6	-2	4	18.321	19.000	-4	4	4	6.020	4.564	-2	10	4	41.461	41.155
-1	-7	4	2.133	5.019	7	-1	4	12.922	12.919	-2	4	4	64.300	64.396	0	10	4	4.927	7.227
-3	-7	4	3.079 *	4.551	5	-1	4	22.955	23.458	0	4	4	4.134	7.036	2	10	4	3.778 *	2.671
-5	-7	4	57.169	58.773	3	-1	4	4.431	2.465	2	4	4	10.075	11.685	4	10	4	14.904	14.826
-7	-7	4	14.243	16.063	1	-1	4	53.019	52.922	4	4	4	48.787	47.963	3	11	4	6.868	7.080
-9	-7	4	11.585	12.135	-1	-1	4	6.632	3.478	6	4	4	8.768	8.468	1	11	4	5.220	6.102
-10	-6	4	14.581	13.478	-3	-1	4	9.703	10.900	5	5	4	13.459	13.113	-1	11	4	19.347	19.070
-8	-6	4	12.572	13.750	-5	-1	4	44.615	44.648	3	5	4	23.353	23.070	-3	11	4	8.089	4.290
-6	-6	4	28.539	27.707	-7	-1	4	2.054	2.376	0	6	0	94.882	93.236	-5	11	4	10.616	10.524
0	6	0	94.589	93.236	-9	-1	4	14.420	13.559	1	5	4	35.753	35.361	-7	11	4	13.459	13.384
-4	-6	4	43.365	41.556	-11	-1	4	2.050	1.858	-1	5	4	12.933	13.542	-8	12	4	16.219	15.054
-2	-6	4	43.144	45.561	-10	0	4	10.023	9.082	-3	5	4	17.976	17.689	-6	12	4	10.837	9.355
0	-6	4	57.424	55.089	-8	0	4	38.291	37.867	-5	5	4	10.327	8.628	-4	12	4	8.434	9.268
2	-6	4	33.954	34.100	-6	0	4	55.227	55.029	-7	5	4	26.237	25.902	-2	12	4	17.972	18.659
4	-6	4	19.718	20.142	-4	0	4	4.056	5.867	-9	5	4	14.202	13.862	0	12	4	15.287	15.588
6	-6	4	29.204	27.833	-2	0	4	158.659	161.260	-10	6	4	22.895	23.159	2	12	4	9.061	8.016
5	-5	4	12.493	14.238	0	0	4	41.521	39.880	-8	6	4	11.949	11.644	1	13	4	11.660	13.632
3	-5	4	53.327	50.397	2	0	4	64.814	65.715	-6	6	4	8.261	9.029	-1	13	4	20.240	21.811
1	-5	4	12.234	10.975	4	0	4	55.314	54.479	-4	6	4	43.019	42.548	0	6	0	94.502	93.236
-1	-5	4	31.979	31.354	0	6	0	94.626	93.236	-2	6	4	18.723	19.148	-3	13	4	11.333	11.960
-3	-5	4	21.262	19.556	6	0	4	7.413	8.045	0	6	4	53.015	54.258	-5	13	4	6.725	0.639
-5	-5	4	2.895 *	2.100	7	1	4	15.734	15.546	2	6	4	43.827	44.036	-7	13	4	11.724	12.129
-7	-5	4	45.813	44.357	5	1	4	24.623	24.811	4	6	4	6.587	4.749	-6	14	4	10.060	10.317
-9	-5	4	9.148	7.850	3	1	4	18.787	19.006	6	6	4	30.507	30.404	-4	14	4	18.554	19.948
-10	-4	4	28.002	25.931	1	1	4	66.072	64.553	5	7	4	12.445	12.591	-2	14	4	18.393	17.886
-8	-4	4	26.713	22.973	-1	1	4	32.452	29.641	3	7	4	11.089	11.118	0	14	4	5.744	5.303
-6	-4	4	4.792	5.980	-3	1	4	4.916	0.375	1	7	4	10.049	11.632	2	14	4	4.480	6.585
-4	-4	4	33.226	32.793	-5	1	4	62.362	61.168	-1	7	4	5.614	7.415	-1	15	4	5.013	5.390
-2	-4	4	24.653	24.228	-7	1	4	18.780	17.536	-3	7	4	11.543	11.868	-3	15	4	4.191 *	2.025
0	-4	4	37.082	36.652	-9	1	4	28.772	28.499	0	6	0	94.506	93.236	-5	15	4	3.511	1.006
0	6	0	94.641	93.236	-11	1	4	2.396 *	1.963	-5	7	4	10.000	10.424	-4	14	5	32.287	31.985
2	-4	4	13.575	14.754	-10	2	4	17.398	16.431	-7	7	4	13.751	13.912	-2	14	5	16.774	16.443
4	-4	4	26.106	24.742	-8	2	4	3.834	1.424	-9	7	4	4.367	2.723	0	14	5	5.539	7.859
6	-4	4	15.452	13.768	-6	2	4	4.885	2.150	-10	8	4	15.253	12.356	1	13	5	7.694	6.867
7	-3	4	30.274	30.250	-4	2	4	59.170	57.988	-8	8	4	7.191	7.700	-1	13	5	20.548	19.782
5	-3	4	31.566	31.628	-2	2	4	39.561	38.924	-6	8	4	5.205	5.728	-3	13	5	29.287	28.778
3	-3	4	5.866	3.649	0	2	4	43.808	43.065	-4	8	4	55.024	55.415	-5	13	5	13.462	13.312
1	-3	4	97.416	96.907	2	2	4	16.910	16.464	-2	8	4	39.551	39.781	-6	12	5	21.066	20.860
-1	-3	4	36.632	37.305	4	2	4	16.759	16.474	0	8	4	38.165	39.107	-4	12	5	17.578	17.794
-3	-3	4	37.667	39.211	6	2	4	22.719	22.311	2	8	4	19.651	20.814	0	6	0	94.465	93.236
-5	-3	4	77.777	76.274	0	6	0	94.563	93.236	4	8	4	3.534 *	2.156	-2	12	5	27.678	27.353
-7	-3	4	11.855	10.580	5	3	4	10.008	9.552	5	9	4	7.319	6.896	0	12	5	14.549	15.305
-9	-3	4	25.182	25.256	3	3	4	14.532	14.726	3	9	4	20.608	20.873	2	12	5	10.560	8.473
-11	-3	4	19.369	19.322	1	3	4	28.888	29.258	1	9	4	19.418	20.001	3	11	5	13.413	13.410
-10	-2	4	4.059	3.023	-1	3	4	30.582	30.132	-1	9	4	42.839	43.749	1	11	5	17.811	16.706
-8	-2	4	38.175	36.197	-3	3	4	22.948	22.833	-3	9	4	11.198	13.842	-1	11	5	15.246	14.549
-6	-2	4	50.593	51.670	-5	3	4	6.872	8.004	-5	9	4	12.982	12.760	-3	11	5	8.085	5.643
-4	-2	4	55.062	52.592	-7	3	4	11.273	11.355	-7	9	4	17.112	17.900	-5	11	5	10.811	10.570
-2	-2	4	57.146	56.166	-9	3	4	5.685	3.806	-9	9	4	21.040	21.318	-7	11	5	14.885	13.526
0	-2	4	61.679	60.321	-11	3	4	11.761	12.171	-8	10	4	4.619	5.862	-8	10	5	5.208	5.263
2	-2	4	45.693	44.956	-10	4	4	23.917	23.919	0	6	0	94.484	93.236	-6	10	5	20.567	19.930
0	6	0	94.578	93.236	-8	4	4	32.201	32.363	-6	10	4	13.278	11.491	-4	10	5	18.002	19.809

(18)

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	10	5	2.546	3.625	1	3	5	23.027	21.769	6	-2	5	6.624	6.625	3	-9	5	6.729	5.846
0	10	5	15.137	14.618	-1	3	5	57.597	58.698	5	-3	5	33.627	32.815	4	-9	5	26.853	23.921
2	10	5	11.709	11.986	-3	3	5	31.307	31.292	3	-3	5	16.301	15.371	-1	-9	5	28.089	26.207
3	9	5	34.401	33.629	-5	3	5	53.549	53.569	1	-3	5	5.648	4.501	-3	-9	5	37.852	36.595
1	9	5	21.104	21.118	-7	3	5	28.156	27.952	-1	-3	5	83.962	84.475	-5	-9	5	29.234	29.660
-1	9	5	6.282	6.024	-9	3	5	17.300	16.927	-3	-3	5	3.391	0.493	-7	-9	5	2.430 *	0.577
-3	9	5	69.989	70.706	-11	3	5	17.416	17.345	-5	-3	5	77.045	76.547	-9	-9	5	31.585	31.367
-5	9	5	7.600	4.791	-10	2	5	4.898	0.725	0	6	0	94.705	93.236	-8	-10	5	3.954	3.446
0	6	0	94.472	93.236	-8	2	5	18.243	18.530	-7	-3	5	48.483	48.735	-6	-10	5	4.931	5.542
-7	9	5	9.471	8.677	-6	2	5	17.244	16.799	-9	-3	5	3.184 *	4.800	-4	-10	5	7.052	2.065
-9	9	5	35.550	35.775	-4	2	5	13.188	12.974	-11	-3	5	37.563	37.824	-2	-10	5	3.466 *	4.595
-8	8	5	27.409	28.611	-2	2	5	31.288	31.461	-10	-4	5	16.658	15.726	0	-10	5	9.917	9.360
-6	8	5	27.473	26.353	0	2	5	19.196	18.769	-8	-4	5	3.075 *	0.008	2	-10	5	4.168	4.578
-4	8	5	15.460	13.745	2	2	5	7.886	5.791	-6	-4	5	32.231	32.761	4	-10	5	7.612	5.251
-2	8	5	35.445	34.429	4	2	5	22.351	22.183	-4	-4	5	45.520	47.021	3	-11	5	2.452	6.180
0	8	5	23.703	23.008	6	2	5	3.440	3.282	-2	-4	5	34.476	34.849	1	-11	5	18.881	19.663
2	8	5	14.217	13.897	5	1	5	39.140	37.936	0	-4	5	27.597	29.198	-1	-11	5	7.067	9.927
4	8	5	23.383	22.014	3	1	5	4.510	3.847	2	-4	5	36.557	36.622	0	6	0	94.810	93.236
3	7	5	2.651 *	3.688	0	6	0	94.476	93.236	4	-4	5	19.433	19.826	-3	-11	5	14.976	16.354
1	7	5	26.016	25.507	1	1	5	26.714	27.030	5	-5	5	3.522	2.128	-5	-11	5	8.866	8.122
-1	7	5	14.086	10.056	-1	1	5	81.592	81.872	3	-5	5	13.030	13.075	-7	-11	5	3.714 *	0.552
-3	7	5	16.526	16.670	-3	1	5	37.546	38.692	1	-5	5	48.427	50.024	-8	-12	5	9.103	8.447
-5	7	5	14.386	11.965	-5	1	5	52.437	54.443	-1	-5	5	3.192 *	2.140	-6	-12	5	25.223	24.822
-7	7	5	15.268	15.238	-7	1	5	36.613	35.080	-3	-5	5	43.178	43.195	-4	-12	5	15.133	15.453
-9	7	5	17.953	17.113	-9	1	5	11.596	11.371	-5	-5	5	20.248	19.524	-2	-12	5	28.783	29.574
-10	6	5	23.575	24.120	-11	1	5	38.194	38.760	-7	-5	5	7.559	5.858	0	-12	5	4.052 *	4.476
-3	6	5	20.811	20.522	-10	0	5	42.828	41.782	-9	-5	5	35.914	37.642	2	-12	5	6.234	6.054
-6	6	5	73.357	73.863	-8	0	5	31.660	32.566	-10	-6	5	20.225	20.333	1	-13	5	23.655	24.053
-4	6	5	25.700	25.658	-6	0	5	33.810	38.901	0	6	0	94.555	93.236	-1	-13	5	23.631	22.529
0	6	0	94.525	93.236	-4	0	5	108.862	108.533	-8	-6	5	14.003	13.360	-3	-13	5	7.507	10.024
-2	6	5	71.761	72.605	-2	0	5	21.532	21.796	-6	-6	5	26.143	26.742	-5	-13	5	4.116 *	1.459
0	6	5	57.882	37.998	0	0	5	44.949	46.126	-4	-6	5	52.050	50.529	-7	-13	5	22.313	21.199
2	6	5	9.940	7.260	2	0	5	49.106	47.507	-2	-6	5	15.933	18.128	-6	-14	5	4.044 *	0.234
4	6	5	36.252	35.678	4	0	5	5.062	5.454	0	-6	5	24.502	24.508	-4	-14	5	8.986	8.499
5	5	5	12.828	12.751	6	0	5	27.424	26.949	2	-6	5	17.277	17.223	-2	-14	5	4.217 *	1.910
3	5	5	29.384	29.093	5	-1	5	12.565	11.925	4	-6	5	11.314	12.040	0	-14	5	9.636	10.352
1	5	5	39.508	38.861	3	-1	5	3.192 *	2.128	5	-7	5	4.559	3.200	-1	-15	5	13.421	14.649
-1	5	5	44.765	44.440	1	-1	5	11.558	10.048	3	-7	5	3.537 *	2.062	-3	-15	5	4.273 *	2.456
-3	5	5	75.216	75.804	-1	-1	5	34.093	33.587	1	-7	5	14.946	13.292	0	6	0	94.694	93.236
-5	5	5	31.675	33.459	0	6	0	94.521	93.236	-1	-7	5	38.922	37.371	-5	-15	5	9.384	8.296
-7	5	5	4.465	1.045	-3	-1	5	8.126	5.362	-3	-7	5	25.783	24.756	-4	-14	6	17.604	17.425
-9	5	5	42.820	43.184	-5	-1	5	10.116	10.822	-5	-7	5	2.655 *	7.665	-2	-14	6	19.294	20.123
-10	4	5	27.987	27.926	-7	-1	5	20.935	20.599	-7	-7	5	16.737	17.011	-1	-13	6	29.835	29.841
-8	4	5	33.950	34.060	-9	-1	5	5.704	5.386	-9	-7	5	12.952	11.508	-3	-13	6	6.662	3.974
-6	4	5	10.199	10.608	-11	-1	5	12.749	11.683	-10	-8	5	2.531 *	1.857	-5	-13	6	21.649	21.399
-4	4	5	68.374	68.381	-10	-2	5	38.858	39.478	-8	-8	5	20.090	20.279	-6	-12	6	21.705	21.416
-2	4	5	7.225	5.307	-8	-2	5	35.100	35.072	-6	-8	5	30.596	36.889	-4	-12	6	5.490	2.666
0	4	5	41.878	43.065	-6	-2	5	28.648	26.977	-4	-8	5	30.139	26.792	-2	-12	6	14.454	11.764
2	4	5	37.702	37.558	-4	-2	5	63.109	64.375	-2	-8	5	49.910	49.070	0	-12	6	20.845	21.556
4	4	5	9.031	10.127	-2	-2	5	7.585	8.828	0	6	0	94.675	93.236	1	-11	6	29.621	28.699
0	6	0	94.533	93.236	0	-2	5	47.071	47.468	0	-8	5	13.338	11.304	-1	-11	6	7.030	8.999
5	3	5	27.101	27.217	2	-2	5	27.394	27.026	2	-8	5	4.732	6.392	-3	-11	6	55.682	55.362
3	3	5	27.537	27.296	4	-2	5	3.203 *	1.724	4	-8	5	23.248	23.019	-5	-11	6	3.376	6.798

H	K	L	F(CBS)	E(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(CBS)	F(CALC)
1	3	7	21.228	20.609	-6	-4	7	9.440	8.740	-1	-9	8	8.438	5.240	1	1	8	24.142	23.734
-1	3	7	23.688	24.511	-4	-4	7	2.895	6.354	-3	-9	8	20.432	19.988	-1	1	8	34.563	34.370
-3	3	7	33.169	34.172	-2	-4	7	28.498	28.827	-5	-9	8	20.353	20.255	-3	1	8	28.505	29.298
-5	3	7	33.365	32.810	0	-4	7	21.344	21.092	0	6	0	93.965	93.236	-5	1	8	7.477	8.861
0	6	0	94.052	93.236	2	-4	7	3.898 *	0.529	-7	-9	8	3.781	1.556	-7	1	8	23.074	29.984
-7	3	7	23.106	23.585	3	-5	7	3.627	2.976	-8	-8	8	8.081	4.633	-9	1	8	31.048	31.717
-9	3	7	17.893	18.628	1	-5	7	35.077	35.461	-6	-8	8	19.583	20.522	-8	2	8	11.333	12.209
-10	2	7	4.568	5.759	-1	-5	7	21.825	22.196	-4	-8	8	8.551	11.953	-6	2	8	9.551	9.730
-8	2	7	26.380	25.827	-3	-5	7	20.098	18.754	-2	-8	8	17.946	18.721	-4	2	8	14.587	15.834
-5	2	7	6.838	4.508	-5	-5	7	35.652	36.943	0	-8	8	13.312	11.651	-2	2	8	8.216	6.519
-4	2	7	3.665 *	1.566	-7	-5	7	10.451	9.691	-1	-7	8	30.071	30.150	0	2	8	4.131 *	0.876
-2	2	7	31.359	32.585	-9	-5	7	24.521	26.419	-3	-7	8	10.946	11.593	1	3	8	4.225 *	0.475
0	2	7	8.002	5.541	-8	-6	7	4.435	4.349	-5	-7	8	7.383	5.567	0	6	0	94.232	93.236
2	2	7	12.662	13.051	-6	-6	7	21.089	20.628	-7	-7	8	30.909	30.913	-1	3	8	7.582	6.131
3	-1	7	34.611	32.829	0	6	0	94.285	93.236	-8	-6	8	3.293	1.040	-3	3	8	4.041	1.210
1	1	7	13.935	12.169	-4	-6	7	30.616	30.676	-6	-6	8	6.588	3.404	-5	3	8	10.360	7.690
-1	1	7	42.599	42.183	-2	-6	7	3.547 *	7.789	-4	-6	8	7.251	10.996	-7	3	8	17.568	17.290
-3	1	7	12.970	12.820	0	-6	7	17.656	16.687	-2	-6	8	12.722	9.649	-9	3	8	3.520	3.852
-5	1	7	14.026	14.734	2	-6	7	12.910	14.720	1	-5	8	16.534	16.125	-6	4	8	6.699	5.475
-7	1	7	43.793	43.893	1	-7	7	23.530	24.074	-1	-5	8	5.565	0.635	-6	4	8	4.570	4.059
-9	1	7	9.193	7.169	-1	-7	7	4.946	2.996	-3	-5	8	5.697	6.407	-4	4	8	6.789	5.438
-10	0	7	34.735	34.127	-3	-7	7	6.891	7.027	-5	-5	8	8.385	7.697	-2	4	8	6.789	5.793
-8	0	7	9.437	9.824	-5	-7	7	38.560	38.055	-7	-5	8	4.765	2.907	0	4	8	4.131 *	0.396
-6	0	7	40.165	39.466	-7	-7	7	11.044	10.947	0	6	0	93.943	93.236	-1	5	8	37.052	37.168
-4	0	7	52.035	52.297	-9	-7	7	7.709	8.648	-9	-5	8	7.026	5.359	-3	5	8	13.432	11.530
0	5	0	94.157	93.236	-8	-8	7	38.449	38.621	-8	-4	8	4.611	4.994	-5	5	8	5.434	4.756
-2	0	7	2.234 *	8.200	-6	-8	7	15.233	16.030	-6	-4	8	16.891	16.459	-7	5	8	25.644	26.272
0	0	7	37.364	36.574	-4	-8	7	8.503	10.437	-4	-4	8	9.523	9.331	-9	5	8	16.222	17.035
2	0	7	16.320	17.205	-2	-8	7	49.876	49.461	-2	-4	8	15.415	15.137	-8	6	8	23.980	24.771
3	-1	7	8.798	7.728	0	-8	7	9.114	7.712	0	-4	8	4.517	4.812	-6	6	8	4.123 *	2.781
1	-1	7	4.149	0.755	2	-8	7	20.620	20.410	1	-3	8	16.448	14.910	-4	6	8	15.006	12.391
-1	-1	7	14.517	13.007	1	-9	7	17.300	17.543	-1	-3	8	49.869	49.920	-2	6	8	4.641	1.464
-3	-1	7	9.151	7.840	-1	-9	7	6.057	1.271	-3	-3	8	4.067 *	4.889	0	6	8	10.300	9.600
-5	-1	7	2.460	0.968	-3	-9	7	4.187	4.179	-5	-3	8	3.958 *	2.618	0	6	0	1.523 *	93.236
-7	-1	7	9.547	11.430	-5	-9	7	35.629	36.022	-7	-3	8	33.290	33.521	-1	7	8	11.630	11.427
-9	-1	7	10.505	9.492	0	6	0	94.026	93.236	-9	-3	8	30.143	30.069	-3	7	8	7.315	1.826
-10	-2	7	37.206	38.700	-7	-9	7	3.872 *	2.521	-8	-2	8	11.618	11.318	-5	7	8	2.482 *	6.420
-8	-2	7	12.700	11.989	-8	-10	7	12.020	11.961	-6	-2	8	4.412	4.483	-7	7	8	7.897	6.692
-6	-2	7	27.508	28.845	-6	-10	7	16.305	16.834	-4	-2	8	15.486	12.635	-6	8	8	4.225 *	0.512
-4	-2	7	36.564	36.937	-4	-10	7	9.850	8.132	-2	-2	8	8.186	9.345	-4	8	8	5.598	10.018
-2	-2	7	5.764	8.940	-2	-10	7	9.992	8.689	0	-2	8	9.756	10.876	-2	8	8	7.488	8.641
0	-2	7	34.435	35.298	0	-10	7	5.813	6.910	1	-1	8	7.642	5.472	-3	9	8	7.229	4.479
2	-2	7	14.818	14.184	-1	-11	7	19.760	20.676	-1	-1	8	4.138 *	5.664	-5	9	8	17.000	16.292
3	-3	7	35.407	34.784	-3	-11	7	3.290	3.634	-3	-1	8	5.392	2.448	-4	6	9	23.173	22.883
1	-3	7	13.192	11.571	-5	-11	7	35.507	36.924	0	6	0	94.074	93.236	-3	5	9	14.333	13.461
-1	-3	7	31.878	30.447	-7	-11	7	7.567	6.911	-5	-1	8	6.305	4.315	-5	5	9	20.875	20.334
0	6	0	94.067	93.236	-6	-12	7	4.262	5.187	-7	-1	8	3.860 *	3.303	-7	5	9	3.132 *	4.982
-3	-3	7	37.371	39.015	-4	-12	7	4.266 *	3.549	-9	-1	8	4.097	4.965	-6	4	9	25.426	25.748
-5	-3	7	3.556 *	2.667	-2	-12	7	23.800	24.076	-8	0	8	5.178	2.676	-4	4	9	16.940	16.337
-7	-3	7	53.128	54.768	-3	-13	7	17.878	16.971	-6	0	8	12.065	12.044	-2	4	9	12.426	12.335
-9	-3	7	5.851	4.161	-6	-10	8	4.258 *	1.386	-4	0	8	19.486	19.328	-3	3	9	17.095	17.821
-10	-4	7	13.244	13.987	-4	-10	8	2.629	7.039	-2	0	8	9.279	7.324	-5	3	9	26.913	27.335
-8	-4	7	25.332	25.739	-2	-10	8	6.245	5.910	0	0	3	3.440 *	5.447	-7	3	9	18.160	17.862

SUENO, PREWITT, AND PAPKE - HIGH ALBITE - 300 DEG. C

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H	K	L	F(OBS)	F(CALC)
-3	2	9	18.115	17.602
0	6	0	94.735	93.236
-6	2	9	16.245	15.240
-4	2	9	6.076	0.473
-2	2	9	15.212	15.882
-1	1	9	6.910	5.608
-3	1	9	41.626	40.813
-5	1	9	4.149 *	1.426
-7	1	9	19.763	20.012
-8	0	9	10.357	9.920
-6	0	9	38.577	39.262
-4	0	9	25.028	27.541
-2	0	9	15.441	16.194
-1	-1	9	2.629 *	5.422
-3	-1	9	6.091	4.153
-5	-1	9	4.258 *	0.425
-7	-1	9	4.119 *	3.305
-8	-2	9	8.821	7.009
-6	-2	9	36.155	37.780
-4	-2	9	26.196	26.371
-2	-2	9	14.127	15.092
-1	-3	9	4.318 *	0.800
0	6	0	94.029	93.236
-3	-3	9	47.229	48.213
-5	-3	9	16.252	16.634
-7	-3	9	24.161	24.991
-8	-4	9	19.009	19.356
-6	-4	9	5.062	7.688
-4	-4	9	7.657	7.567
-2	-4	9	6.016	6.385
-3	-5	9	18.355	17.506
-5	-5	9	27.499	28.647
-7	-5	9	18.205	18.355
-6	-6	9	28.006	29.117
-4	-6	9	22.373	23.653
-2	-6	9	10.064	9.691
-3	-7	9	16.988	17.684
-5	-7	9	12.963	13.249

ATOM	PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
	EXTINCTION CORRECTION	0.0		0.0		
	SCALE FACTOR 1	2.6630	0.0003	2.6633	0.00647	0.04
ATOM 1	NA1	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.2747549	-0.0000020	0.2747529	0.0003569	-0.01
	Y	0.0059290	-0.0000034	0.0059256	0.0003465	-0.01
	Z	0.1348100	0.0000047	0.1348147	0.0005792	0.01
	BETA11	0.0111400	-0.0000027	0.0111373	0.0004607	-0.01
	BETA22	0.0199200	0.0000032	0.0199232	0.0004495	0.01
	BETA33	0.0484600	0.0000157	0.0484757	0.0012080	0.01
	BETA12	0.0015300	0.0000042	0.0015342	0.0003544	0.01
	BETA13	0.0046000	-0.0000103	0.0045897	0.0006000	-0.02
	BETA23	-0.0177700	-0.0000085	-0.0177735	0.0006045	-0.01
ATOM 2	T10	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.0088570	-0.0000001	0.0088569	0.0001310	-0.00
	Y	0.1673990	-0.0000003	0.1673986	0.0000752	-0.00
	Z	0.2163799	0.0000005	0.2163805	0.0001487	0.00
	BETA11	0.0060300	-0.0000018	0.0060782	0.0001589	-0.01
	BETA22	0.0020400	-0.0000001	0.0020399	0.0000529	-0.00
	BETA33	0.0067500	-0.0000029	0.0067471	0.0002069	-0.01
	BETA12	-0.0003500	-0.0000013	-0.0003513	0.0000694	-0.02
	BETA13	0.0033400	0.0000017	0.0033417	0.0001480	0.01
	BETA23	0.0004000	0.0000041	0.0004041	0.0000794	0.05
ATOM 3	T1M	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.0053770	-0.0000002	0.0053768	0.0001295	-0.00
	Y	0.6154960	0.0000002	0.6154961	0.0000761	0.00
	Z	0.2284180	0.0000007	0.2284187	0.0001466	0.00
	BETA11	0.0059100	0.0000008	0.0059108	0.0001601	0.00
	BETA22	0.0021800	-0.0000025	0.0021775	0.0000535	-0.05
	BETA33	0.0062000	-0.0000012	0.0061988	0.0002054	-0.01
	BETA12	0.0008200	-0.0000030	0.0008170	0.0000702	-0.04
	BETA13	0.0030800	-0.0000039	0.0030761	0.0001485	-0.03
	BETA23	0.0006000	-0.0000025	0.0005975	0.0000792	-0.03
ATOM 4	T20	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.6919160	-0.0000001	0.6919159	0.0001290	-0.00
	Y	0.1095530	-0.0000004	0.1095526	0.0000736	-0.00
	Z	0.3241990	0.0000003	0.3241993	0.0001536	0.00
	BETA11	0.0054000	0.0000004	0.0054004	0.0001559	0.00
	BETA22	0.0016900	0.0000034	0.0016934	0.0000510	0.07
	BETA33	0.0086100	0.0000037	0.0086137	0.0002210	0.02
	BETA12	-0.0000400	-0.0000012	-0.0000412	0.0000677	-0.02
	BETA13	0.0028000	-0.0000031	0.0027969	0.0001512	-0.02
	BETA23	0.0003900	-0.0000045	0.0003855	0.0000805	-0.06

ATM 5 T2H EQUIPOINT FRACTION = 1.000

OCCUPANCY SPECIES 2	0.75000		0.75000		
OCCUPANCY SPECIES 4	0.25000		0.25000		
TOTAL OCCUPANCY (FIXED) =	1.00000				
X	0.6977130	0.0000004	0.6877133	0.0001296	0.00
Y	0.8784870	-0.0000000	0.8784870	-0.0000741	0.00
Z	0.3525320	0.0000006	0.3525326	0.0001539	0.00
BETA11	0.0054800	0.0000003	0.0054808	0.0001560	0.00
BETA22	0.0016900	0.0000015	0.0016915	0.0000502	0.03
BETA33	0.0086200	0.0000014	0.0086214	0.0002196	0.01
BETA12	0.0003200	-0.0000013	0.0003187	0.0000670	-0.02
BETA13	0.0031200	0.0000026	0.0031226	0.0001504	0.02
BETA23	0.0005000	-0.0000030	0.0004970	0.0000796	-0.04

ATOM 6 OAl EQUIPOINT FRACTION = 1.000

OCCUPANCY SPECIES 3	1.00000		1.00000		
X	0.0045600	0.0000004	0.0045604	0.0004488	0.00
Y	0.1358960	0.0000002	0.1358961	0.0002377	0.00
Z	0.9373620	0.0000001	0.9873620	0.0004562	0.00
BETA11	0.0159300	0.0000018	0.0159318	0.0006422	0.00
BETA22	0.0037300	-0.0000038	0.0037262	0.0001830	-0.02
BETA33	0.0113600	-0.0000016	0.0113584	0.0006735	-0.00
BETA12	0.0006300	-0.0000046	0.0006254	0.0002665	-0.02
BETA13	0.0082300	-0.0000046	0.0082254	0.0005540	-0.01
BETA23	0.0005500	-0.0000000	0.0005500	0.0002752	-0.00

ATM 7 OA2 EQUIPOINT FRACTION = 1.000

OCCUPANCY SPECIES 3	1.00000		1.00000		
X	0.5750530	-0.0000014	0.5950515	0.0003576	-0.00
Y	0.9924050	-0.0000008	0.9924042	0.0002002	-0.00
Z	0.2797770	-0.0000013	0.2797757	0.0004373	-0.00
BETA11	0.0076900	-0.0000028	0.0076872	0.0004571	-0.01
BETA22	0.0121000	0.0000030	0.0021030	0.0001430	0.02
BETA33	0.0141100	0.0000040	0.0141140	0.0006778	0.01
BETA12	0.0001900	-0.0000004	0.0001896	0.0001976	-0.00
BETA13	0.0036400	-0.0000044	0.0036356	0.0004565	-0.01
BETA23	0.0009600	-0.0000034	0.0009634	0.0002432	0.01

ATM 8 OBO EQUIPOINT FRACTION = 1.000

OCCUPANCY SPECIES 3	1.00000		1.00000		
X	0.8209810	-0.0000006	0.8209804	0.0004089	-0.00
Y	0.1135899	-0.0000009	0.1135890	0.0002454	-0.00
Z	0.2020590	0.0000006	0.2020596	0.0004987	0.00
BETA11	0.0105100	0.0000020	0.0105120	0.0005404	0.00
BETA22	0.0042800	0.0000032	0.0042832	0.0001919	0.02
BETA33	0.0180700	-0.0000013	0.0180687	0.0008003	-0.00
BETA12	-0.0012700	-0.0000036	-0.0012736	0.0002535	-0.01
BETA13	0.0092700	0.0000024	0.0092724	0.0005624	0.00
BETA23	-0.0003500	-0.0000028	-0.0003528	0.0003083	-0.01

ATM 9 OBM EQUIPOINT FRACTION = 1.000

OCCUPANCY SPECIES 3	1.00000		1.00000		
X	0.8197890	-0.0000001	0.8197889	0.0004328	-0.00
Y	0.8490810	0.0000006	0.8490816	0.0002757	0.00
Z	0.2434240	-0.0000006	0.2434233	0.0005338	-0.00
BETA11	0.0106300	0.0000049	0.0106349	0.0005661	0.01
BETA22	0.0056500	0.0000028	0.0056527	0.0002303	0.01
BETA33	0.0200100	-0.0000007	0.0200093	0.0008775	-0.00
BETA12	0.0019300	-0.0000038	0.0019262	0.0002838	-0.01
BETA13	0.0094400	0.0000037	0.0094437	0.0005991	0.01
BETA23	0.0002500	-0.0000038	0.0002462	0.0003532	-0.01

ATOM 10	OCC	EQUIPOINT FRACTION = 1.000			
		OCCUPANCY SPECIES 3	1.00000	1.00000	
X		0.0189370	-0.0000008	0.0189362	0.0003890 -0.00
Y		0.2932690	-0.0000003	0.2932686	0.0002229 -0.00
Z		0.2747660	-0.0000001	0.2747658	0.0004805 -0.00
BETA11		0.0093300	-0.0000015	0.0093315	0.0005069 0.00
BETA22		0.0024800	-0.0000047	0.0028753	0.0001622 -0.03
BETA33		0.0171600	-0.0000027	0.0171573	0.0007673 -0.00
BETA12		-0.0105600	0.0000023	-0.0005577	0.0002244 0.01
BETA13		0.0055800	-0.0000036	0.0055764	0.0005166 -0.01
BETA23		-0.0007700	0.0000003	-0.0007697	0.0002776 0.00
ATOM 11	OCH	EQUIPOINT FRACTION = 1.000			
		OCCUPANCY SPECIES 3	1.00000	1.00000	
X		0.0224290	0.0000001	0.0224291	0.0003970 0.00
Y		0.6989600	-0.0000004	0.6889595	0.0002238 -0.00
Z		0.2247600	0.0000007	0.224607	0.0004607 0.00
BETA11		0.0100100	-0.0000017	0.0100082	0.0005203 -0.00
BETA22		0.0029000	0.0000016	0.0029016	0.0001632 0.01
BETA33		0.0140300	0.0000040	0.0140340	0.0007146 0.01
BETA12		0.0011000	0.0000005	0.0011005	0.0002282 0.00
BETA13		0.0030400	0.0000023	0.0030423	0.0005005 0.00
BETA23		0.0005400	0.0000025	0.0005425	0.0002682 0.01
ATOM 12	ODD	EQUIPOINT FRACTION = 1.000			
		OCCUPANCY SPECIES 3	1.00000	1.00000	
X		0.1941700	0.0000004	0.1941704	0.0004002 0.00
Y		0.1140610	-0.0000005	0.1140605	0.0002302 -0.00
Z		0.3999789	0.0000003	0.3899792	0.0004399 0.00
BETA11		0.0106500	-0.0000001	0.0106499	0.0005322 -0.00
BETA22		0.0035300	0.0000047	0.0035347	0.0001753 0.03
BETA33		0.0103200	-0.0000023	0.0103177	0.0006473 -0.00
BETA12		0.0014800	-0.0000043	0.0014757	0.0002409 -0.02
BETA13		0.0020900	-0.0000037	0.0020863	0.0004788 -0.01
BETA23		0.0012900	0.0000023	0.0012923	0.0002638 0.01
ATOM 13	ODM	EQUIPOINT FRACTION = 1.000			
		OCCUPANCY SPECIES 3	1.00000	1.00000	
X		0.1382066	-0.0000012	0.1382047	0.0004115 -0.00
Y		0.8587980	-0.0000002	0.8687977	0.0002434 -0.00
Z		0.4234110	-0.0000008	0.4234101	0.0004536 -0.00
BETA11		0.0108400	0.0000024	0.0108424	0.0005525 0.00
BETA22		0.0340200	-0.0000001	0.0040199	0.0001870 -0.00
BETA33		0.0105300	-0.0000040	0.0105260	0.0006649 -0.01
BETA12		-0.0005200	-0.0000023	-0.0005223	0.0002526 -0.01
BETA13		0.0012200	-0.0000060	0.0012140	0.0004885 -0.01
BETA23		-0.0007300	-0.0000007	-0.0007307	0.0002774 -0.00

MAXIMUM SHIFT/ERROR = 0.07

AVERAGE SHIFT/ERROR = 0.01

X

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H	K	L	E(OBS)	E(CALC)	H	K	L	E(OBS)	E(CALC)	H	K	L	E(OBS)	E(CALC)	H	K	L	E(OBS)	E(CALC)
0	-8	4	64.171	65.001	0	6	0	96.238	95.136	-5	3	4	13.679	13.449	-3	9	4	3.514 *	4.016
2	-8	4	22.693	22.143	-4	-2	4	52.457	50.165	-7	3	4	8.102	8.332	-5	9	4	11.31	12.735
4	-8	4	22.224	22.193	-2	-2	4	49.934	49.710	-9	3	4	5.675	6.805	-7	9	4	19.887	20.129
6	-8	4	26.156	26.593	0	-2	4	57.594	55.951	-11	3	4	9.571	9.670	-9	9	4	16.900	17.258
5	-7	4	13.594	14.307	2	-2	4	42.345	42.334	-10	4	4	21.418	20.510	-8	10	4	4.970	5.766
3	-7	4	7.903	10.177	4	-2	4	37.671	36.651	-8	4	4	25.745	24.986	-5	10	4	0.190	6.043
1	-7	4	49.598	51.302	6	-2	4	15.019	15.874	-6	4	4	28.709	29.840	-4	10	4	24.148	25.747
-1	-7	4	3.264 *	2.857	7	-1	4	9.188	9.550	-4	4	4	11.416	10.024	-2	10	4	35.766	35.579
-3	-7	4	3.190 *	2.623	5	-1	4	20.569	20.501	-2	4	4	51.737	61.178	0	10	4	4.900	6.331
-5	-7	4	47.241	49.435	3	-1	4	2.613	0.560	0	4	4	3.050 *	0.991	2	10	4	2.610	0.215
-7	-7	4	12.306	14.405	1	-1	4	52.059	52.467	0	6	0	96.273	95.136	4	10	4	12.898	10.930
9	6	0	96.316	95.136	-1	-1	4	8.487	7.166	2	4	4	12.611	14.449	3	11	4	5.154 *	1.106
-9	-7	4	9.141	8.288	-3	-1	4	3.405	9.001	4	4	4	40.226	39.180	1	11	4	5.536	6.102
-10	-6	4	14.275	12.603	-5	-1	4	44.012	43.834	5	4	4	9.936	8.643	-1	11	4	12.218	11.420
-8	-6	4	9.845	10.765	-7	-1	4	4.721	5.860	5	5	4	13.119	9.176	-3	11	4	7.549	1.818
-6	-6	4	25.750	26.124	-9	-1	4	13.176	12.701	3	5	4	27.743	27.483	-5	11	4	9.422	10.013
-4	-6	4	49.320	59.373	-11	-1	4	3.646 *	1.437	1	5	4	33.398	34.294	-7	11	4	9.327	8.150
-2	-6	4	42.185	43.160	-10	0	4	9.932	9.175	-1	5	4	15.716	15.075	-8	12	4	10.372	9.253
0	-6	4	55.783	55.705	-8	0	4	34.189	33.274	-3	5	4	11.751	12.122	-6	12	4	9.445	8.750
2	-6	4	31.572	31.128	-6	0	4	54.528	54.385	-5	5	4	10.095	9.602	-4	12	4	12.584	13.120
4	-6	4	13.533	19.337	-4	0	4	3.439	5.343	-7	5	4	27.852	27.542	0	6	0	95.518	95.136
6	-6	4	24.234	23.905	0	6	0	96.378	95.136	-9	5	4	12.140	12.603	-2	12	4	14.485	15.526
5	-5	4	12.547	11.148	-2	0	4	154.941	150.330	-10	6	4	18.380	17.292	0	12	4	15.256	15.513
3	-5	4	43.371	47.194	0	0	4	39.840	39.163	-8	6	4	6.185	5.311	2	12	4	9.087	7.918
1	-5	4	14.874	13.206	2	0	4	63.350	63.878	-5	6	4	9.079	10.291	3	13	4	13.130	12.654
-1	-5	4	29.516	28.634	4	0	4	49.492	49.112	-4	6	4	41.067	40.195	1	13	4	14.215	14.749
-3	-5	4	18.080	16.779	6	0	4	5.341	5.909	-2	6	4	23.116	22.271	-1	13	4	17.402	19.150
-5	-5	4	3.038	1.793	7	1	4	12.296	12.443	0	6	4	54.014	54.562	-3	13	4	9.094	7.716
-7	-5	4	42.726	41.189	5	1	4	23.131	23.354	2	6	4	35.752	36.882	-5	13	4	6.621	3.398
-9	-5	4	9.556	2.842	3	1	4	15.969	15.507	4	6	4	5.278	7.923	-7	13	4	12.647	12.592
-10	-4	4	26.257	22.740	1	1	4	63.521	62.590	6	6	4	25.793	25.612	-5	14	4	3.682	9.821
-8	-4	4	21.609	19.462	-1	1	4	21.852	25.949	0	6	0	96.336	95.136	-4	14	4	13.052	13.429
0	6	0	96.300	95.136	-3	1	4	4.771	1.434	5	7	4	9.141	10.331	-2	14	4	19.469	17.930
-6	-4	4	10.563	12.462	-5	1	4	58.560	57.343	3	7	4	10.037	9.704	0	14	4	3.751	4.052
-4	-4	4	32.213	21.376	-7	1	4	15.872	16.181	1	7	4	14.138	14.680	2	14	4	3.735	0.372
-2	-4	4	30.394	29.910	-9	1	4	23.973	24.432	-1	7	4	5.329	7.481	-1	15	4	2.952	1.252
3	-4	4	33.975	33.343	-11	1	4	3.677 *	0.374	-3	7	4	11.003	10.882	-3	15	4	4.374 *	0.264
2	-4	4	15.914	17.472	-10	2	4	13.636	12.030	-5	7	4	12.650	12.427	-5	15	4	4.306 *	1.132
4	-4	4	23.895	22.595	-8	2	4	5.387	3.936	-7	7	4	9.320	9.676	-4	14	5	25.913	27.513
5	-4	4	13.176	12.274	-6	2	4	8.697	6.951	-9	7	4	5.061	2.633	-2	14	5	12.927	13.455
7	-3	4	23.186	23.571	-4	2	4	55.813	54.468	-12	9	4	14.800	12.830	0	14	5	19.301	7.491
5	-3	4	28.191	28.287	-2	2	4	25.305	24.733	-8	8	4	4.343	4.958	0	6	0	95.342	95.156
3	-3	4	3.934 *	2.539	0	6	0	95.323	95.136	-6	8	4	3.318 *	2.617	1	13	5	8.241	5.632
1	-3	4	86.056	85.136	0	2	4	44.814	43.929	-4	8	4	53.936	53.609	-1	13	5	13.532	19.030
-1	-3	4	36.142	35.290	2	2	4	13.442	13.552	-2	8	4	31.357	31.033	-3	13	5	22.025	22.973
-3	-3	4	33.168	34.061	4	2	4	17.344	17.547	0	8	4	39.766	39.155	-5	13	5	11.938	11.355
-5	-3	4	55.963	64.730	6	2	4	19.642	19.212	2	8	4	20.103	21.243	-7	13	5	2.730	0.759
-7	-3	4	3.527	9.251	7	3	4	19.124	18.577	4	8	4	4.818	4.183	-6	12	5	19.611	19.034
-9	-3	4	21.963	22.047	5	3	4	11.926	12.531	5	9	4	5.119	5.552	-4	12	5	11.326	11.596
-11	-3	4	13.901	13.327	3	3	6	12.315	11.992	3	9	4	24.129	24.155	-2	12	5	23.269	24.307
-10	-2	4	5.979	2.815	1	3	4	34.551	33.887	1	9	4	15.318	16.826	0	12	5	12.261	12.739
-8	-2	4	29.017	27.073	-1	3	4	33.177	29.071	-1	9	4	41.348	42.391	2	12	5	5.094	4.828
-6	-2	4	55.291	45.693	-3	3	4	23.155	22.731	0	6	0	96.612	95.136	3	11	5	14.554	14.576

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
1	11	5	16.707	14.049	-10	4	5	21.316	21.313	-9	-1	5	4.331	1.831	-5	-7	5	8.932	11.034
-1	11	5	16.592	12.171	-8	4	5	27.151	27.325	-11	-1	5	12.047	12.423	-7	-7	5	12.993	13.913
-3	11	5	10.746	10.405	-6	4	5	7.579	4.959	-10	-2	5	29.231	29.514	-9	-7	5	10.291	8.381
-5	11	5	9.336	8.551	-4	4	5	52.438	55.532	-8	-2	5	31.534	31.904	-10	-9	5	2.960	4.560
-7	11	5	14.722	14.151	-2	4	5	10.247	9.395	-6	-2	5	29.280	27.874	-8	-8	5	16.767	17.952
-8	10	5	5.976	8.102	0	4	5	37.145	56.323	-4	-2	5	53.359	54.429	-5	-8	5	38.532	37.547
-6	10	5	15.892	16.362	2	4	5	32.986	33.923	-2	-2	5	12.027	13.117	-4	-8	5	25.461	22.444
-4	10	5	13.867	19.436	4	4	5	11.315	12.304	0	-2	5	41.846	42.321	-2	-8	5	46.286	40.299
-2	10	5	5.445	3.109	5	3	5	24.647	25.202	3	6	0	95.460	95.135	0	-8	5	13.044	11.327
0	6	0	95.538	95.130	3	3	5	23.914	23.641	2	-2	5	21.897	22.525	2	-8	5	5.437	4.712
2	10	5	11.575	11.732	1	3	5	22.597	22.190	4	-2	5	3.392 *	0.170	4	-8	5	21.601	20.932
2	10	5	12.401	11.149	-1	3	5	58.613	59.256	5	-2	5	6.255	4.668	3	-9	5	5.715	3.208
3	9	5	24.923	24.590	-3	3	5	25.820	25.736	5	-3	5	21.778	27.025	1	-9	5	24.566	24.182
1	9	5	23.743	22.718	-5	3	5	54.177	54.240	3	-3	5	17.250	16.880	-1	-9	5	23.730	21.837
-1	9	5	4.559	0.730	-7	3	5	27.100	26.195	1	-3	5	7.229	7.122	-3	-9	5	39.560	39.100
-3	9	5	63.447	64.121	-9	3	5	13.792	12.800	-1	-3	5	78.995	79.630	-5	-9	5	25.367	26.933
-5	0	5	9.717	6.344	-11	3	5	17.648	17.154	-2	-2	5	4.527	2.730	-7	-9	5	5.151	1.334
-7	9	5	9.659	8.005	-13	2	5	6.859	4.907	-5	-3	5	72.249	72.261	-9	-9	5	29.273	29.151
-9	9	5	31.073	31.368	-9	2	5	17.776	17.335	-7	-3	5	40.384	41.569	3	6	0	95.448	95.136
-10	9	5	12.493	10.512	0	6	0	96.448	95.136	-9	-3	5	3.276 *	3.382	-8	-10	5	5.788	4.915
-8	8	5	21.951	23.104	-5	2	5	23.748	19.709	-11	-3	5	30.820	31.514	-6	-10	5	3.595 *	3.207
-5	8	5	33.703	29.900	-4	2	5	5.807	4.510	-10	-4	5	13.168	12.714	-4	-10	5	9.853	5.910
-4	8	5	9.418	8.224	-2	2	5	30.300	29.759	-8	-4	5	4.635	3.892	-2	-10	5	3.922 *	3.217
-2	8	5	16.818	30.227	0	2	5	23.946	19.325	-6	-4	5	23.435	26.819	0	-10	5	7.229	8.458
0	8	5	22.080	20.659	2	2	5	9.126	7.133	-4	-4	5	45.168	46.090	2	-10	5	4.058 *	1.584
2	8	5	2.231	9.234	4	2	5	12.135	17.702	-2	-4	5	31.934	32.504	4	-10	5	5.845	4.019
4	8	5	22.056	20.358	6	2	5	3.400	2.594	0	-4	5	27.225	26.238	3	-11	5	4.226 *	1.127
5	7	5	3.090	0.521	5	1	5	28.826	28.226	2	-4	5	32.214	33.007	1	-11	5	18.169	13.235
3	7	5	3.840 *	0.711	3	1	5	5.397	6.715	4	-4	5	18.715	15.773	-1	-11	5	3.120	3.190
1	7	5	19.890	19.957	1	1	5	21.702	21.933	0	6	0	95.523	95.135	-3	-11	5	16.549	16.561
0	6	0	95.491	95.136	-1	1	5	75.657	75.751	6	-4	5	15.595	15.551	-5	-11	5	6.220	7.357
-1	7	5	14.528	15.004	-3	1	5	33.305	33.525	5	-5	5	5.133	0.933	-7	-11	5	7.192	6.144
-3	7	5	7.573	7.146	-5	1	5	48.257	49.499	3	-5	5	12.152	12.710	-9	-12	5	4.241	5.057
-5	7	5	16.479	16.292	-7	1	5	32.343	31.216	1	-5	5	46.092	47.930	-6	-12	5	22.236	23.251
-7	7	5	11.544	11.441	-9	1	5	8.904	10.110	-1	-5	5	3.377 *	3.104	-4	-12	5	13.149	14.358
-9	7	5	11.956	11.440	-11	1	5	31.194	31.151	-3	-5	5	45.176	44.932	-2	-12	5	25.153	25.721
-10	6	5	20.880	21.341	-10	0	5	36.351	35.516	-5	-5	5	16.238	15.447	0	-12	5	4.312 *	1.091
-8	6	5	16.759	17.935	-8	0	5	31.708	32.759	-7	-5	5	6.308	5.337	2	-12	5	8.120	5.256
-6	6	5	63.108	63.358	-6	0	5	34.576	34.547	-9	-5	5	33.858	34.479	1	-13	5	19.770	16.431
-4	6	5	26.142	26.219	-4	0	5	105.811	107.013	-10	-6	5	17.575	16.970	0	6	0	95.674	95.130
-2	6	5	52.403	62.975	0	6	0	96.522	95.136	-8	-6	5	14.878	13.238	-1	-13	5	24.954	22.626
0	6	5	33.441	33.835	-2	0	5	19.275	18.330	-6	-6	5	23.296	28.404	-3	-13	5	5.098	8.377
2	6	5	7.735	6.370	0	0	5	53.088	45.743	-4	-6	5	45.150	44.531	-5	-13	5	4.358 *	1.458
4	6	5	30.247	29.804	2	0	5	44.327	43.176	-2	-6	5	20.619	21.498	-7	-13	5	17.579	18.300
5	5	5	8.744	7.999	4	0	5	5.520	6.162	0	-6	5	23.735	23.920	-6	-14	5	6.314	0.195
3	5	5	23.453	23.916	6	0	5	24.597	23.619	2	-6	5	14.107	13.920	-4	-14	5	13.228	10.175
1	5	5	39.034	36.539	5	-1	5	11.712	10.835	4	-6	5	12.522	12.570	-2	-14	5	5.944	0.559
-1	5	5	35.261	35.013	3	-1	5	3.318 *	3.302	5	-7	5	3.868 *	1.947	0	-14	5	8.615	9.819
-3	5	5	67.279	58.052	1	-1	5	9.834	9.381	3	-7	5	3.739 *	2.355	-1	-15	5	7.100	9.222
-5	5	5	22.613	24.584	-1	-1	5	38.099	37.679	1	-7	5	12.623	10.079	-3	-15	5	4.074	4.512
-7	5	5	3.225	1.632	-3	-1	5	10.142	8.517	0	6	0	95.358	95.130	-5	-15	5	6.559 *	0.546
0	6	0	95.650	95.135	-5	-1	5	14.411	16.081	-1	-7	5	33.967	32.530	-4	-14	6	15.949	14.293
-9	5	5	39.105	37.936	-7	-1	5	21.270	20.518	-3	-7	5	23.895	22.737	-2	-14	6	15.408	15.592

SUENO, PREWITT, AND PAPKE - HIGH ALBITE - 600 DEG. C

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-1	-13	6	21.795	23.916	-5	-5	6	9.877	5.633	-10	2	6	12.343	12.674	2	8	6	3.396	4.542
-3	-13	6	8.659	6.357	-7	-5	6	13.996	13.917	-8	2	6	8.763	8.830	1	9	5	4.417	7.003
-5	-13	6	18.969	18.439	-9	-5	6	12.530	11.116	-6	2	6	19.965	20.301	-1	9	5	7.408	5.058
-5	-12	6	15.533	16.106	-10	-4	5	15.057	14.943	-4	2	6	8.849	9.178	-3	9	6	25.598	26.584
-4	-12	6	8.853	1.762	-8	-4	6	17.945	16.579	-2	2	6	6.504	4.421	-5	9	5	23.238	29.052
-2	-12	6	10.228	7.592	-5	-4	5	25.176	23.153	0	2	6	20.833	19.248	-7	9	6	8.685	7.044
0	-12	5	19.781	18.617	-4	-4	6	9.975	9.782	0	6	0	95.230	95.136	-9	9	5	2.450 *	2.711
0	6	0	25.343	95.136	-2	-4	5	12.518	11.120	2	2	6	2.765	1.624	-8	10	5	15.428	17.452
1	-11	5	22.528	22.267	0	-4	6	28.859	27.035	4	2	6	13.157	13.175	-6	10	6	10.734	9.666
-1	-11	6	5.636	7.131	2	-4	6	15.090	14.623	3	3	6	4.744	4.230	-4	10	5	4.822	3.312
-3	-11	6	42.929	42.215	4	-4	5	3.331	7.750	1	3	6	7.559	6.678	-2	10	6	19.073	19.497
-5	-11	6	4.771	4.876	3	-3	6	12.752	13.658	-1	3	6	3.790 *	6.205	0	10	5	10.734	10.509
-7	-11	6	19.042	16.072	1	-3	6	18.029	17.586	-3	3	6	3.533	3.340	2	10	6	12.199	12.005
-9	-10	5	13.799	13.965	-1	-3	6	45.229	45.411	-5	3	6	3.568 *	4.409	1	11	6	3.198	1.220
-5	-10	6	5.538	3.915	-3	-3	6	36.721	37.498	-7	3	6	3.361 *	4.343	-1	11	6	4.475 *	2.150
-4	-10	6	20.483	20.405	-5	-3	6	43.299	42.144	-9	3	6	7.108	6.954	-3	11	6	11.439	9.359
-2	-10	6	23.934	24.014	-7	-3	6	4.830	5.138	-10	4	6	15.444	15.935	0	6	0	9.296	95.436
0	-10	6	5.242	4.390	0	6	0	96.425	95.136	-9	4	6	15.077	13.776	-5	11	5	10.212	9.953
2	-10	6	13.056	12.929	-9	-3	6	17.320	17.328	-6	4	6	8.467	7.330	-7	11	6	8.448	6.903
3	-9	6	22.154	20.401	-10	-2	6	3.525 *	3.518	-4	4	6	3.599 *	6.160	-6	12	6	4.300 *	0.732
1	-9	6	16.019	16.625	-8	-2	6	15.062	14.711	-2	4	6	5.772	9.565	-4	12	5	5.515	0.215
-1	-9	6	7.361	6.548	-6	-2	5	15.961	17.211	0	4	6	10.567	11.036	-2	12	6	4.475 *	3.093
-3	-9	5	13.222	44.908	-4	-2	6	15.256	13.634	2	4	6	16.824	15.054	0	12	6	0.586	8.318
-5	-9	6	3.883 *	1.046	-2	-2	6	18.282	17.839	4	4	6	2.859	4.406	-1	13	5	5.379	0.335
-7	-9	5	5.543	7.697	0	-2	6	19.961	19.925	3	5	6	30.458	29.681	-3	13	6	11.186	13.024
-9	-9	6	12.039	11.080	2	-2	6	22.352	22.256	1	5	6	8.630	8.433	-5	13	6	11.727	12.329
-8	-9	6	5.485	1.159	4	-2	6	15.038	14.196	-1	5	5	19.777	14.271	-4	12	7	15.794	15.512
-5	-8	5	33.477	39.776	5	-1	6	13.963	13.285	0	6	0	96.479	95.135	-1	11	7	15.658	16.328
7	6	0	96.538	99.136	3	-1	6	2.360	0.846	-3	5	6	15.766	35.829	-3	11	7	13.710	13.353
-4	-8	6	11.559	12.507	1	-1	6	8.837	10.454	-5	5	6	26.101	23.828	-5	11	7	2.999	0.139
-2	-8	6	17.157	17.503	-1	-1	6	15.505	14.388	-7	5	6	12.502	13.768	-6	10	7	4.312 *	3.057
0	-8	6	39.696	40.031	-3	-1	6	17.842	17.459	-9	5	6	12.339	10.612	-4	10	7	13.320	12.442
2	-8	6	11.494	8.016	-5	-1	6	22.002	22.273	-10	6	6	8.826	7.781	-2	10	7	12.206	12.182
3	-7	6	17.304	12.703	-7	-1	6	3.389 *	2.273	-9	6	6	10.174	18.999	0	10	7	4.650 *	4.079
1	-7	6	4.396	3.617	-9	-1	6	4.101	1.475	-6	6	6	13.250	11.056	-1	9	7	4.101 *	0.226
-1	-7	6	18.075	20.514	-11	-1	6	2.654	2.028	-4	6	6	11.081	9.249	-3	9	7	27.222	26.111
-3	-7	6	43.170	44.957	-10	0	6	11.716	13.145	-2	6	6	5.624	5.714	-5	9	7	34.625	34.222
-5	-7	6	25.048	27.137	-8	0	6	22.037	21.051	0	6	6	31.797	30.305	0	6	0	96.557	95.130
-7	-7	5	3.579	1.093	0	6	0	95.392	95.136	2	6	6	9.043 *	1.735	-7	9	7	5.698	5.124
-7	-7	6	15.116	15.404	-6	0	6	8.257	9.310	4	6	6	11.159	10.472	-6	8	7	25.045	26.381
-10	-6	5	2.731	1.652	-4	0	6	17.172	15.963	3	7	6	4.148 *	2.929	-6	8	7	17.612	17.515
-8	-6	6	5.104	1.362	-2	0	6	38.520	36.671	1	7	6	4.035 *	2.649	-4	8	7	17.750	16.376
-5	-6	6	8.978	8.683	0	0	5	4.755	4.303	-1	7	5	4.191	1.031	-2	8	7	29.336	29.337
-4	-6	6	11.248	9.039	2	0	6	30.719	30.240	-3	7	6	3.891 *	8.357	0	8	7	15.160	14.655
-2	-6	6	16.857	13.451	4	0	6	6.909	5.070	-5	7	6	7.202	3.506	1	7	7	5.671	5.352
0	-6	5	23.553	20.737	3	1	6	19.116	19.591	-7	7	6	2.948 *	0.912	-1	7	7	4.043	5.027
2	-5	6	5.556	7.123	1	1	6	4.561	5.935	-9	7	5	4.504	5.185	-7	7	7	4.140 *	0.549
4	-6	6	-11.065	10.775	-1	1	6	21.989	19.656	-8	8	6	10.870	10.475	-5	7	7	9.488	6.137
3	-5	6	27.108	26.457	-3	1	6	67.085	68.391	0	6	0	96.374	95.136	-7	7	7	5.644	0.803
0	6	0	96.658	95.136	-5	1	6	38.162	37.106	-6	8	6	15.852	16.412	-9	7	7	7.712	3.390
1	-5	6	13.293	12.731	-7	1	6	9.784	10.361	-4	8	6	13.760	13.819	-8	6	7	37.557	30.341
-1	-5	6	7.887	3.518	-9	1	6	15.534	16.039	-2	8	6	4.016 *	2.065	-6	6	7	34.734	34.919
-3	-5	6	29.161	27.894	-11	1	6	11.603	13.216	0	8	6	22.536	22.719	-4	6	7	22.660	23.318

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-2	6	7	47.975	47.447	-9	-1	7	7.903	5.439	-7	-9	7	9.109 *	0.701	-7	-3	8	25.017	25.048
0	6	7	11.283	10.303	-10	-2	7	27.829	29.137	-8	-10	7	8.380	9.034	-9	-3	8	24.958	25.059
2	6	7	17.632	17.750	-9	-2	7	13.270	13.414	-6	-10	7	13.644	13.620	-9	-2	8	7.778	8.492
1	5	7	41.659	41.499	-6	-2	7	24.047	25.232	-4	-10	7	10.773	9.435	-6	-2	8	6.927	4.195
-1	5	7	3.498 *	0.616	-6	-2	7	31.241	30.702	0	6	0	96.393	95.136	-4	-2	2	11.649	10.225
0	6	0	96.580	95.136	-2	-2	7	5.528	11.013	-2	-10	7	3.178	0.175	-2	-2	8	7.716	7.855
-3	5	7	18.529	17.851	0	-2	7	28.055	28.499	0	-10	7	6.594	6.493	0	-2	8	8.724	9.711
-5	5	7	32.761	36.069	2	-2	7	12.736	11.202	-1	-11	7	17.953	18.476	1	-1	8	3.926	3.829
-7	5	7	14.967	15.097	3	-3	7	31.329	30.045	-3	-11	7	8.674	8.491	-1	-1	8	8.086	9.192
-9	5	7	32.354	33.007	1	-3	7	9.005	7.385	-5	-11	7	-29.344	29.754	-3	-1	8	4.771	2.036
-10	4	7	21.899	22.247	-1	-3	7	29.397	20.103	-7	-11	7	8.892	8.397	-5	-1	8	5.799	4.599
-8	4	7	3.782 *	1.811	-3	-3	7	32.277	34.547	-5	-12	7	3.104	6.022	-7	-1	8	2.052 *	6.221
-6	4	7	13.683	14.833	-5	-3	7	5.624	4.934	-4	-12	7	4.125	2.609	-7	-1	8	3.498	1.716
-4	4	7	22.664	22.214	-7	-3	7	44.972	46.203	-2	-12	7	21.927	21.731	-10	0	8	3.949 *	2.209
-2	4	7	7.977	6.764	-9	-3	7	5.280	2.621	-3	-13	7	15.396	16.159	0	6	0	96.475	95.130
0	4	7	25.184	24.649	0	6	0	96.230	95.136	-6	-10	8	4.522 *	0.445	-8	0	8	5.702	4.338
2	4	7	2.231 *	4.595	-10	-6	7	13.546	14.045	-4	-10	8	7.170	7.542	-5	0	8	12.711	9.957
3	3	7	13.808	18.970	-8	-4	7	20.527	21.212	-2	-10	8	2.902	3.284	-4	0	8	17.614	19.125
1	3	7	14.092	15.699	-6	-4	7	6.902	6.856	-1	-9	8	5.201	0.691	-2	0	8	5.754	7.227
-1	3	7	25.130	25.597	-4	-4	7	5.583	1.839	-3	-9	8	15.208	16.818	0	0	8	2.343	6.598
-3	3	7	28.771	29.400	-2	-4	7	25.084	26.571	-5	-9	8	14.785	-14.914	1	1	8	19.900	16.495
-5	3	7	27.396	27.310	0	-4	7	21.086	19.673	-7	-9	9	5.485	5.169	-1	1	8	29.211	29.753
-7	3	7	23.421	23.130	2	-6	7	2.745	1.707	-9	-9	8	4.304 *	1.405	-3	1	9	22.352	23.408
-9	3	7	13.207	13.419	3	-5	7	6.874	1.801	-6	-8	8	17.379	17.004	-5	1	8	9.070 *	6.434
-10	2	7	3.549	1.032	1	-5	7	31.524	33.412	-4	-8	8	7.591	10.553	-7	1	8	21.827	24.710
-3	2	7	23.011	22.424	-1	-5	7	18.680	20.152	2	6	0	96.304	95.136	-9	1	9	25.441	25.022
0	6	9	96.487	95.136	-3	-5	7	14.010	16.570	-2	-8	8	15.766	15.176	-8	2	8	7.759	8.933
-6	2	7	8.919	8.743	-5	-5	7	35.459	36.082	0	-8	8	9.394	8.717	-6	2	8	8.351	6.609
-4	2	7	3.825 *	2.508	-7	-5	7	7.217	9.810	-1	-7	9	24.479	24.912	-4	2	8	0.004	11.993
-2	2	7	27.857	26.745	-9	-5	7	23.061	23.731	-3	-7	8	9.662	8.482	-2	2	8	5.305	2.131
0	2	7	7.186	6.529	-8	-6	7	3.670	6.853	-5	-7	8	5.455	2.118	0	2	8	3.759	1.220
2	2	7	11.829	12.316	-5	-6	7	10.735	19.407	-7	-7	8	24.273	24.427	1	3	9	5.538	1.704
3	1	7	23.483	27.550	-4	-6	7	25.808	26.013	-8	-6	8	2.803 *	0.463	-1	3	8	4.536	0.419
1	1	7	10.555	10.050	-2	-6	7	6.284	10.877	-5	-6	8	5.902	3.875	-3	3	8	2.921 *	2.339
-1	1	7	35.248	34.608	0	-6	7	14.995	13.943	-4	-6	9	4.238	1.784	-5	2	8	8.740	6.330
-3	1	7	13.749	13.003	2	-6	7	17.955	12.230	-2	-6	8	12.175	9.372	0	6	0	95.273	95.150
-5	1	7	11.360	13.330	0	6	0	96.541	95.130	0	-6	8	6.796	7.187	-7	3	8	12.826	9.533
-7	1	7	34.006	37.582	1	-7	7	17.603	19.659	1	-5	8	15.529	14.333	-9	3	8	9.148	7.429
-9	1	7	3.035	0.733	-1	-7	7	3.914	2.250	-1	-5	8	5.597	5.155	-8	4	8	5.349	5.932
-10	0	7	33.250	32.102	-3	-7	7	4.615	3.000	-3	-5	8	5.734	6.011	-6	4	8	2.921	5.199
-9	0	7	7.792	8.274	-5	-7	7	22.979	29.115	-5	-5	8	3.381	4.545	-4	4	8	7.630	6.745
-5	0	7	35.195	35.323	-7	-7	7	10.255	9.513	-7	-5	8	7.474	3.414	-2	4	8	5.985	3.505
-4	0	7	49.752	49.215	-9	-7	7	7.439	7.640	-9	-5	8	7.618	6.085	0	4	8	4.358 *	0.792
-2	0	7	3.938 *	5.195	-8	-9	7	34.228	34.157	-8	-4	8	5.690	5.125	-1	5	8	31.525	32.058
0	0	7	35.315	34.075	-6	-8	7	15.404	16.795	-6	-4	8	13.620	13.639	-3	5	8	12.047	9.528
2	0	7	12.791	13.085	-4	-8	7	7.558	8.922	-4	-4	8	10.290	10.282	-5	5	8	5.725	4.937
3	-1	7	9.615	9.004	-2	-9	7	44.604	44.132	0	6	0	75.532	95.135	-7	5	8	21.799	23.211
0	6	0	95.109	95.136	0	-8	7	6.839	6.609	-2	-4	8	8.744	11.809	-9	5	8	14.925	14.183
1	-1	7	2.646 *	2.389	2	-8	7	17.464	17.928	0	-4	8	4.296 *	1.875	-8	6	8	19.551	18.509
-1	-1	7	14.302	13.805	1	-9	7	17.449	17.230	1	-3	8	13.094	12.911	-6	6	8	9.270 *	3.939
-3	-1	7	9.577	8.485	-1	-9	7	6.859	2.744	-1	-3	8	32.056	39.411	-4	6	8	12.452	10.858
-5	-1	7	3.743 *	3.063	-3	-9	7	3.583	4.667	-3	-3	8	3.351	5.359	-2	6	8	4.389 *	2.007
-7	-1	7	12.489	14.665	-5	-9	7	33.538	34.899	-5	-3	8	4.120 *	0.570	0	6	8	7.825	6.118

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J	K	L	E(DBS)	E(CALC)	J	K	L	E(DBS)	E(CALC)
-1	7	3	4.241	3.701	-7	-5	9	15.611	15.282
-3	7	8	4.212	0.500	-5	-6	9	22.637	23.220
-5	7	9	4.362 *	2.920	-4	-6	9	19.751	20.479
0	6	0	95.230	95.136	-2	-6	9	11.548	10.950
-7	7	8	3.096	1.305	-3	-7	9	13.114	13.584
-5	8	9	4.421 *	1.206	-5	-7	9	9.654	9.603
-4	9	8	6.425	8.001					
-2	8	8	4.627 *	5.872					
-3	9	9	5.655	0.094					
-5	9	8	11.969	11.740					
-6	6	9	8.582	9.239					
-6	6	9	20.374	19.593					
-3	5	9	12.070	10.309					
-5	5	9	20.144	18.120					
-7	5	9	5.512	1.951					
-6	4	9	22.341	21.990					
-6	4	9	12.970	13.349					
-2	4	9	9.293	8.313					
-3	3	9	13.715	19.327					
-5	3	9	21.320	21.997					
-7	3	9	16.565	16.475					
-9	2	9	15.248	15.392					
-5	2	9	7.214	6.393					
-4	2	9	4.822	3.524					
0	6	0	95.273	95.136					
-2	2	9	12.709	12.851					
-1	1	9	4.549 *	3.636					
-3	1	9	35.564	35.351					
-5	1	9	4.343 *	1.792					
-7	1	9	15.467	16.033					
-9	0	9	5.102	7.015					
-6	0	9	35.783	36.957					
-4	0	9	23.618	24.610					
-2	0	9	15.416	14.092					
-1	-1	9	2.243	3.292					
-3	-1	9	9.386	7.995					
-5	-1	9	4.386 *	0.387					
-7	-1	9	4.335 *	4.284					
-9	-2	9	9.745	8.328					
-5	-2	9	29.176	29.543					
-4	-2	9	21.040	21.559					
-2	-2	9	15.260	14.291					
-1	-3	9	5.968	2.769					
-3	-3	9	40.984	41.393					
-5	-3	9	13.005	15.251					
0	6	0	95.140	95.136					
-7	-3	9	20.845	21.849					
-3	-4	9	15.595	15.224					
-6	-4	9	8.148	9.630					
-4	-4	9	3.052 *	4.239					
-2	-4	9	2.976 *	4.579					
-3	-5	9	13.461	11.920					
-5	-5	9	24.093	25.041					

ATOM	PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
	EXTINCTION CORRECTION	0.0		0.0		
	SCALE FACTOR 1	2.5675	-0.0000	2.5675	0.00645	-0.01
ATOM 1	N41	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.2761230	-0.0000011	0.2761219	0.0004125	-0.00
	Y	0.0037040	-0.0000023	0.0037017	0.0003895	-0.01
	Z	0.1373529	0.0000025	0.1373554	0.0006529	0.00
	BETA11	0.0153600	-0.0000041	0.0153559	0.0005600	-0.01
	BETA22	0.0226700	0.0000047	0.0226747	0.0005353	0.01
	BETA33	0.0579000	0.0000056	0.0579956	0.0014728	0.00
	BETA12	0.0007910	0.0000017	0.0007917	0.0004299	0.00
	BETA13	0.0074400	-0.0000013	0.0074387	0.0007325	-0.00
	BETA23	-0.0166500	-0.0000046	-0.0166545	0.0007121	-0.01
ATOM 2	T10	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.0087350	-0.0000025	0.0087845	0.0001371	-0.00
	Y	0.1697140	0.0000032	0.1697142	0.0000797	0.00
	Z	0.2174430	0.0000006	0.2174485	0.0001563	0.00
	BETA11	0.0078600	0.0000030	0.0078630	0.0001689	0.02
	BETA22	0.0026910	0.0000032	0.0026932	0.0000565	0.06
	BETA33	0.0088700	-0.0000002	0.0088698	0.0002191	-0.00
	BETA12	-0.0005910	0.0000009	-0.0005891	0.0000745	0.01
	BETA13	0.0040400	-0.0000038	0.0040352	0.0001558	-0.02
	BETA23	0.0003300	0.0000027	0.0003327	0.0000851	0.03
ATOM 3	T1M	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.00061360	0.0000005	0.00061365	0.0001358	0.00
	Y	0.8164790	-0.0000003	0.8164785	0.0000796	-0.00
	Z	0.2274570	0.0000037	0.2274575	0.0001551	0.00
	BETA11	0.0079210	0.0000044	0.0079244	0.0001691	0.03
	BETA22	0.0027100	-0.0000026	0.0027074	0.0000565	-0.05
	BETA33	0.0084330	-0.0000042	0.0084255	0.0002156	-0.02
	BETA12	0.0009800	-0.0000004	0.0009796	0.0000749	-0.01
	BETA13	0.0040220	0.0000008	0.0040208	0.0001564	0.01
	BETA23	0.0005700	-0.0000006	0.0005694	0.0000646	-0.01
ATOM 4	T20	EQUIPOINT FRACTION = 1.000				
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.4931300	0.0000005	0.4931304	0.0001349	0.00
	Y	0.1100500	-0.0000004	0.1100505	0.0000768	-0.00
	Z	0.3200910	0.0000004	0.3200913	0.0001618	0.00
	BETA11	0.0071100	-0.0000018	0.0071082	0.0001634	-0.01
	BETA22	0.0021200	0.0000042	0.0021342	0.0000526	0.08
	BETA33	0.0111500	0.0000024	0.0111524	0.0002355	0.01
	BETA12	-0.0000300	-0.0000015	-0.0000315	0.0000711	-0.02
	BETA13	0.0036000	-0.0000039	0.0035961	0.0001595	-0.02
	BETA23	0.0004000	-0.0000009	0.0003991	0.0000860	-0.01

ATOM 5	T24	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 2	0.75000		0.75000	
		OCCUPANCY SPECIES 4	0.25000		0.25000	
		TOTAL OCCUPANCY (FIXED) =	1.00000			
	X		0.6901900	0.0000002	0.6901901	0.0001345
	Y		0.8795522	-0.0000003	0.8795535	0.0000776
	Z		0.3510080	-0.0000000	0.3510079	0.0001535
	BFTA11		0.0070500	-0.0000043	0.0070457	0.0001641
	BFTA22		0.0022220	0.000021	0.0022221	0.0000531
	BFTA33		0.0114500	0.0000005	0.0114505	0.0002360
	BETA12		0.0003500	0.0000042	0.0003542	0.0000714
	BETA13		0.0039200	0.0000024	0.0039224	0.0001599
	BETA23		0.0105900	0.0000043	0.0005943	0.0000856
ATOM 6	DA1	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 3	1.00000		1.00000	
	X		0.0394500	-0.0000001	0.0394599	0.0004816
	Y		0.1370590	-0.0000004	0.1370555	0.0002547
	Z		0.9696140	0.0000006	0.9896145	0.0004691
	BFTA11		0.0199300	-0.0000016	0.0199284	0.0007303
	BFTA22		0.0048300	0.0000050	0.0048350	0.0002061
	BFTA33		0.0124600	0.0000041	0.0124641	0.0007062
	BETA12		0.0007100	-0.0000011	0.0007089	0.0003042
	BETA13		0.0096100	-0.0000021	0.0096079	0.0006063
	BETA23		0.0007000	0.0000036	0.0007036	0.0003023
ATOM 7	DA2	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 3	1.00000		1.00000	
	X		0.5992200	-0.0000016	0.5992274	0.0003818
	Y		0.9938270	0.0000011	0.9938281	0.0002112
	Z		0.2810100	0.0000020	0.2810120	0.0004705
	BFTA11		0.0100900	0.0000010	0.0100910	0.0004963
	BFTA22		0.0026300	-0.0000050	0.0026250	0.0001514
	BFTA33		0.0180100	0.0000078	0.0180178	0.0007562
	BETA12		0.0001000	0.0000060	0.0001060	0.0002150
	BETA13		0.0041900	-0.0000004	0.0041896	0.0000508
	BETA23		0.0012900	-0.0000042	0.0012858	0.0002580
ATOM 8	DR0	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 3	1.00000		1.00000	
	X		0.8217410	0.0000003	0.8217413	0.0004550
	Y		0.1185300	0.0000011	0.1185400	0.0002766
	Z		0.2070500	0.0000021	0.2070520	0.0005633
	BFTA11		0.0134500	0.0000042	0.0139542	0.0006287
	BFTA22		0.0058200	0.0000009	0.0058209	0.0002333
	BFTA33		0.0243900	0.0000016	0.0243916	0.0009673
	BFTA12		-0.0020500	0.0000013	-0.0020487	0.0003026
	BETA13		0.0119200	-0.0000009	0.0119191	0.0006700
	BETA23		0.0002700	-0.0000006	0.0002194	0.0003774
ATOM 9	DRM	EQUIPOINT FRACTION = 1.000				
		OCCUPANCY SPECIES 3	1.00000		1.00000	
	X		0.8207850	-0.0000001	0.8207859	0.0004659
	Y		0.8522150	-0.0000002	0.8522158	0.0002978
	Z		0.2401730	-0.0000005	0.2401775	0.0005806
	BFTA11		0.0135500	-0.0000016	0.0135582	0.0006329
	BFTA22		0.0069300	-0.0000013	0.0069287	0.0002625
	BFTA33		0.0250300	0.0000020	0.0250320	0.0010022
	BETA12		0.0024400	0.0000046	0.0024445	0.0003209
	BETA13		0.0121400	-0.0000017	0.0121383	0.0006789
	BETA23		0.0001900	0.0000053	0.0001953	0.0004053

ATOM 10 OCO		EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 3					
X		1.00000		1.00000			
Y		0.0209440	-0.0000015	0.0209525	0.0004245	-0.00	
Z		0.2955379	-0.0000013	0.2955365	0.0002371	-0.01	
BETA11		0.700240	-0.0000004	0.2709235	0.0005138	-0.00	
BETA22		0.0035800	0.0000017	0.0035817	0.0001763	0.01	
BETA33		0.0207100	0.0000040	0.0207140	0.0008496	0.00	
BETA12		-0.0009500	-0.0000001	-0.0009501	0.0002516	-0.00	
BETA13		0.0071900	-0.0000001	0.0073899	0.0005779	-0.00	
BETA23		-0.0007800	-0.0000045	-0.0007845	0.0003071	-0.01	
ATOM 11 OCM		EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 3					
X		1.00000		1.00000			
Y		0.0234390	-0.0000000	0.0236390	0.0004228	-0.00	
Z		0.4899400	0.0000007	0.6899407	0.0002377	0.00	
BETA11		0.2310150	0.0000001	0.2310150	0.0005113	0.00	
BETA22		0.0120900	0.0000009	0.0120809	0.0005649	0.00	
BETA33		0.0035400	-0.0000052	0.0035348	0.0001780	-0.03	
BETA12		0.0199200	0.0000025	0.0199225	0.0008432	0.00	
BETA13		0.0013400	0.0000015	0.0013415	0.0002498	0.01	
BETA23		0.0004600	0.0000017	0.0004617	0.0005640	0.00	
		0.0008200	-0.0000013	0.0008167	0.0003074	-0.00	
ATOM 12 ODN		EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 3					
X		1.00000		1.00000			
Y		0.1926550	-0.0000000	0.1926550	0.0004376	-0.00	
Z		0.1157590	0.0000003	0.1157592	0.0002573	0.00	
BETA11		0.397979	-0.0000005	0.3927974	0.0004748	-0.00	
BETA22		0.0137300	-0.0000023	0.0137277	0.0006057	-0.00	
BETA33		0.0049600	0.0000034	0.0049634	0.0002088	0.02	
BETA12		0.0131500	-0.0000040	0.0131560	0.0007207	-0.01	
BETA13		0.0016100	-0.0000042	0.0016058	0.0002812	-0.02	
BETA23		0.0026600	-0.0000014	0.0026585	0.0005373	-0.00	
		0.0012100	-0.0000013	0.0012087	0.0003089	-0.00	
ATOM 13 ODM		EQUIPOINT FRACTION = 1.000					
		OCCUPANCY SPECIES 3					
X		1.00000		1.00000			
Y		0.1800730	-0.0000000	0.1800779	0.0004608	-0.00	
Z		0.8697340	-0.0000007	0.8697333	0.002723	-0.00	
BETA11		0.4195430	0.0000012	0.4195442	0.0004946	0.00	
BETA22		0.0145300	0.0000009	0.0145309	0.0006351	0.00	
BETA33		0.0054300	-0.0000021	0.0054279	0.002218	-0.01	
BETA12		0.0134300	0.0000010	0.0134310	0.0007434	0.00	
BETA13		0.0008900	0.0000017	-0.0008983	0.0022971	0.01	
BETA23		-0.0016300	-0.0000001	0.0016299	0.0005492	-0.00	
		-0.0011800	-0.0000046	-0.0011846	0.0003227	-0.01	

MAXIMUM SHIFT/ERROR = 0.08

AVERAGE SHIFT/ERROR = 0.01

X

H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
4	2	3	2.538	3.704	-9	-3	3	11.412	11.423	-1	-9	3	12.790	11.799	0	-16	4	7.336	0.923
6	2	3	3.810	2.701	-11	-3	3	17.803	18.269	-3	-9	3	53.629	53.049	0	6	0	98.448	95.017
8	2	3	4.937	5.875	0	6	0	98.609	95.817	-5	-9	3	13.082	11.141	1	-15	4	4.060	2.602
7	1	3	2.170 *	3.335	-10	-4	3	7.412	8.619	-7	-9	3	22.507	21.835	-1	-15	4	15.176	15.027
5	1	3	21.265	21.071	-8	-4	3	28.016	28.057	-9	-9	3	14.290	13.771	-3	-15	4	14.315	14.032
3	1	3	28.380	28.400	-6	-4	3	46.900	48.426	-8	-10	3	9.624	8.549	-5	-15	4	4.467 *	2.182
1	1	3	79.158	76.771	-4	-4	3	19.375	20.596	-6	-10	3	3.598 *	4.726	-6	-14	4	13.010	12.447
-1	1	3	36.657	32.268	-2	-4	3	19.735	18.272	-4	-10	3	7.543	8.383	-4	-14	4	3.098	4.108
-3	1	3	46.018	43.003	0	-4	3	57.748	57.224	-2	-10	3	19.939	18.909	-2	-14	4	25.033	26.596
-5	1	3	48.963	47.765	2	-4	3	80.501	79.630	0	-10	3	18.477	16.538	0	-14	4	4.149	1.933
-7	1	3	15.705	15.319	4	-4	3	35.826	36.275	2	-10	3	7.759	4.813	2	-14	4	21.358	20.446
-9	1	3	6.819	6.861	6	-4	3	3.242 *	3.662	4	-10	3	4.111	2.951	3	-13	4	15.481	14.924
-11	1	3	18.273	18.072	7	-5	3	11.128	10.957	0	6	0	98.389	95.817	1	-13	4	21.121	21.100
0	6	0	98.668	95.817	5	-5	3	12.675	12.667	6	-10	3	2.534 *	1.001	-1	-13	4	4.255 *	0.897
-10	0	3	9.815	9.166	3	-5	3	45.243	46.896	5	-11	3	7.018	5.292	-3	-13	4	4.975	2.147
-8	0	3	47.747	47.100	1	-5	3	17.053	15.212	3	-11	3	13.408	13.792	-5	-13	4	20.922	20.882
-6	0	3	3.077 *	3.873	-1	-5	3	10.099	14.013	1	-11	3	4.933	2.796	-7	-13	4	12.518	13.490
-4	0	3	106.089	103.161	-3	-5	3	47.573	48.606	-1	-11	3	17.604	17.771	-8	-12	4	8.832	7.881
-2	0	3	14.192	17.745	-5	-5	3	35.161	35.003	-3	-11	3	15.447	16.007	-6	-12	4	4.327	2.453
0	0	3	37.975	36.064	-7	-5	3	33.673	31.979	-5	-11	3	3.632 *	3.028	-4	-12	4	21.197	19.735
2	0	3	51.625	50.278	-9	-5	3	14.252	14.191	-7	-11	3	19.624	20.002	-2	-12	4	10.370	9.757
4	0	3	25.033	25.678	-10	-6	3	11.912	12.638	-8	-12	3	11.917	11.090	0	-12	4	30.677	30.459
6	0	3	4.390	3.152	-8	-6	3	8.141	5.910	-6	-12	3	26.262	26.545	0	6	0	98.550	95.817
8	0	3	14.468	14.626	0	6	0	98.418	95.817	-4	-12	3	6.335	4.741	2	-12	4	4.988	1.920
7	-1	3	6.738	6.518	-6	-6	3	14.158	14.432	-2	-12	3	2.259 *	5.217	4	-12	4	5.903	3.991
5	-1	3	13.091	12.414	-4	-6	3	39.361	37.050	0	-12	3	25.927	26.723	5	-11	4	9.484	9.870
3	-1	3	23.952	24.198	-2	-6	3	3.178 *	3.796	2	-12	3	24.761	25.362	3	-11	4	31.677	30.697
1	-1	3	56.524	53.644	0	-6	3	14.095	12.727	4	-12	3	16.735	17.787	1	-11	4	3.310	6.112
-1	-1	3	22.036	18.607	2	-6	3	8.281	9.404	3	-13	3	10.065	9.455	-1	-11	4	24.147	25.379
-3	-1	3	28.037	26.321	4	-6	3	3.606	1.811	1	-13	3	6.895	2.894	-3	-11	4	24.711	24.748
-5	-1	3	32.237	31.526	6	-6	3	4.369	4.501	-1	-13	3	19.062	19.057	-5	-11	4	2.534 *	5.448
-7	-1	3	4.352	2.302	7	-7	3	8.552	9.738	-3	-13	3	19.057	20.805	-7	-11	4	26.821	26.017
-9	-1	3	3.928	6.338	5	-7	3	2.365 *	3.401	-5	-13	3	24.350	25.313	-8	-10	4	11.408	11.195
-11	-1	3	12.946	12.188	3	-7	3	31.940	31.541	0	6	0	98.283	95.817	-6	-10	4	6.916	5.403
0	6	0	98.664	95.817	1	-7	3	20.774	19.690	-7	-13	3	6.916	5.589	-4	-10	4	5.056	4.055
-10	-2	3	15.871	15.196	-1	-7	3	25.075	25.416	-6	-14	3	2.615	1.289	-2	-10	4	34.322	35.490
-8	-2	3	28.588	29.027	-3	-7	3	31.228	29.183	-4	-14	3	4.433	3.610	0	-10	4	3.954 *	0.979
-6	-2	3	22.079	20.764	-5	-7	3	24.257	23.794	-2	-14	3	12.773	12.122	2	-10	4	7.776	8.938
-4	-2	3	28.597	27.809	-7	-7	3	12.328	11.919	0	-14	3	6.255	4.200	4	-10	4	7.662	6.628
-2	-2	3	8.378	9.402	-9	-7	3	8.658	6.581	2	-14	3	16.892	16.508	5	-9	4	4.428	5.544
0	-2	3	8.675	8.384	-10	-8	3	19.672	18.524	4	-14	3	9.751	5.703	3	-9	4	37.534	38.738
2	-2	3	29.770	28.463	-8	-8	3	3.250	1.918	3	-15	3	4.674 *	2.133	1	-9	4	7.620	6.138
4	-2	3	13.463	12.901	-6	-8	3	51.951	51.073	1	-15	3	7.217	9.558	-1	-9	4	53.053	53.217
6	-2	3	2.394 *	2.168	-4	-8	3	14.616	14.438	-1	-15	3	5.318	1.543	0	6	0	98.249	95.817
8	-2	3	5.505	4.126	0	6	0	98.435	99.817	-3	-15	3	7.611	6.362	-3	-9	4	43.204	43.218
7	-3	3	3.276 *	1.199	-2	-8	3	13.180	13.236	-5	-15	3	4.098	4.513	-5	-9	4	3.577 *	2.252
5	-3	3	26.537	25.867	0	-8	3	59.562	58.633	-4	-16	3	9.861	10.466	-7	-9	4	30.885	32.519
3	-3	3	26.651	28.052	2	-8	3	35.996	34.057	-2	-16	3	4.539 *	1.375	-9	-9	4	3.119	1.047
1	-3	3	41.547	40.674	4	-8	3	22.812	22.598	0	-16	3	14.921	14.208	-10	-8	4	24.507	23.930
-1	-3	3	9.247	5.119	6	-8	3	4.666	3.670	2	-16	3	11.671	10.546	-8	-8	4	7.615	6.598
-3	-3	3	14.574	14.504	5	-9	3	20.371	19.527	-1	-17	3	11.226	12.197	-6	-8	4	25.715	26.443
-5	-3	3	81.823	80.690	3	-9	3	16.930	16.168	-4	-16	4	3.318	4.047	-4	-8	4	55.464	56.169
-7	-3	3	21.625	22.065	1	-9	3	14.900	14.884	-2	-16	4	24.003	23.667	-2	-8	4	3.505 *	4.454

SUENO, PREWITT, AND PAPKE - HIGH ALRITE - 750 DEG. C

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	-8	4	60.715	62.058	0	6	0	98.473	95.817	-5	3	4	18.642	18.280	-3	9	4	3.695 *	4.202
2	-8	4	22.448	21.402	-4	-2	4	50.904	48.850	-7	3	4	4.666	6.221	-5	9	4	11.425	11.546
4	-8	4	19.655	19.519	-2	-2	4	43.331	43.459	-9	3	4	7.577	9.010	-7	9	4	20.286	22.007
6	-8	4	26.020	25.566	0	-2	4	55.286	53.708	-11	3	4	8.738	8.558	-9	9	4	13.608	13.741
5	-7	4	12.429	11.596	2	-2	4	39.365	39.252	-10	4	4	20.151	19.298	-8	10	4	6.090	5.645
3	-7	4	4.886	7.723	4	-2	4	32.669	31.889	-8	4	4	21.918	20.594	-6	10	4	7.319	6.583
1	-7	4	42.501	45.176	6	-2	4	13.743	13.917	-6	4	4	29.042	29.169	-4	10	4	17.883	17.222
-1	-7	4	3.174	1.504	7	-1	4	8.043	7.853	-4	4	4	14.269	14.234	-2	10	4	32.648	32.376
-3	-7	4	4.526	0.718	5	-1	4	19.375	19.346	-2	4	4	59.274	57.755	0	10	4	4.810	5.452
-5	-7	4	40.250	42.299	3	-1	4	3.060 *	2.519	0	4	4	3.098 *	3.932	2	10	4	3.996 *	2.104
-7	-7	4	8.395	9.775	1	-1	4	52.116	51.890	0	6	0	98.702	95.817	4	10	4	9.709	8.502
0	6	0	98.334	95.817	-1	-1	4	10.226	9.190	2	4	4	14.158	15.948	3	11	4	5.539	4.026
-9	-7	4	5.759	6.116	-3	-1	4	7.675	6.849	4	4	4	34.534	33.643	1	11	4	7.806	6.573
-10	-6	4	12.735	11.888	-5	-1	4	44.658	44.379	6	4	4	9.649	9.070	-1	11	4	8.086	5.105
-8	-6	4	9.124	9.908	-7	-1	4	7.505	8.429	5	5	4	7.403	7.287	-3	11	4	6.725	1.629
-6	-6	4	25.876	24.948	-9	-1	4	13.480	12.749	3	5	4	31.406	31.185	-5	11	4	8.776	10.019
-4	-6	4	38.742	38.407	-11	-1	4	3.187	1.555	1	5	4	31.232	30.874	-7	11	4	8.306	3.471
-2	-6	4	40.780	41.936	-10	0	4	9.065	8.568	-1	5	4	18.138	16.837	-8	12	4	7.734	6.727
0	-6	4	56.036	55.313	-8	0	4	31.410	30.486	-3	5	4	7.645	7.049	-6	12	4	7.878	6.942
2	-6	4	29.067	29.611	-6	0	4	54.367	54.384	-5	5	4	9.806	9.603	-4	12	4	15.214	15.076
4	-6	4	18.256	18.475	-4	0	4	3.776	5.197	-7	5	4	29.457	28.840	0	6	0	98.736	95.817
6	-6	4	22.320	22.142	0	6	0	98.440	95.817	-9	5	4	10.874	10.907	-2	12	4	13.887	13.362
5	-5	4	8.226	9.221	-2	0	4	154.692	156.217	-10	6	4	15.676	14.600	0	12	4	15.074	17.027
3	-5	4	46.149	46.280	0	0	4	38.962	37.778	-8	6	4	4.403	1.272	2	12	4	8.238	7.319
1	-5	4	16.205	14.904	2	0	4	62.499	62.907	-6	6	4	10.696	11.818	3	13	4	14.023	13.564
-1	-5	4	27.749	27.139	4	0	4	45.806	45.401	-4	6	4	39.221	38.791	1	13	4	15.184	15.775
-3	-5	4	15.206	15.000	6	0	4	5.882	5.039	-2	6	4	26.308	25.544	-1	13	4	15.612	16.975
-5	-5	4	6.119	4.591	7	1	4	10.082	10.067	0	6	4	54.489	54.279	-3	13	4	7.281	4.683
-7	-5	4	40.123	39.309	5	1	4	22.490	22.382	2	6	4	32.038	32.183	-5	13	4	7.814	5.973
-9	-5	4	4.166	0.741	3	1	4	13.442	12.752	4	6	4	9.836	9.681	-7	13	4	11.446	12.972
-10	-4	4	22.376	20.344	1	1	4	61.736	61.185	6	6	4	23.638	23.091	-6	14	4	11.090	9.603
-8	-4	4	18.964	17.450	-1	1	4	24.499	22.331	0	6	0	98.876	95.817	-4	14	4	10.535	8.773
0	6	0	98.304	95.817	-3	1	4	2.233	2.353	5	7	4	7.221	9.082	-2	14	4	19.909	16.659
-6	-4	4	14.993	16.630	-5	1	4	55.875	54.932	3	7	4	8.957	7.922	0	14	4	3.000	2.817
-4	-4	4	28.927	29.039	-7	1	4	15.379	14.603	1	7	4	16.871	17.693	2	14	4	2.890 *	3.891
-2	-4	4	35.758	34.536	-9	1	4	21.600	21.339	-1	7	4	7.001	7.288	1	15	4	11.705	14.098
0	-4	4	30.313	29.952	-11	1	4	3.742 *	0.539	-3	7	4	9.488	9.677	-1	15	4	2.882	2.300
2	-4	4	17.975	19.244	-10	2	4	10.611	9.170	-5	7	4	14.222	14.921	-3	15	4	4.551 *	2.876
4	-4	4	22.664	21.822	-8	2	4	7.467	5.827	-7	7	4	7.035	6.949	-5	15	4	7.984	2.730
6	-4	4	11.836	11.240	-6	2	4	11.934	11.529	-9	7	4	3.598	2.233	-2	16	4	14.680	13.302
7	-3	4	19.413	20.277	-4	2	4	53.494	52.507	-10	8	4	13.688	13.637	-3	15	5	9.705	8.476
5	-3	4	25.384	25.951	-2	2	4	14.065	13.318	-8	8	4	3.899	2.649	0	6	0	98.401	95.817
3	-3	4	3.352	0.933	0	6	0	98.257	95.817	-6	8	4	4.530	1.030	-4	14	5	24.978	24.855
1	-3	4	78.251	76.548	0	2	4	46.149	45.083	-4	8	4	53.672	53.836	-2	14	5	11.544	11.542
-1	-3	4	32.555	32.393	2	2	4	20.396	20.614	-2	8	4	25.605	24.049	0	14	5	8.319	1.020
-3	-3	4	30.982	31.615	4	2	4	19.668	19.036	0	8	4	41.242	40.004	1	13	5	4.691 *	5.769
-5	-3	4	58.142	55.629	6	2	4	17.218	16.971	2	8	4	20.329	21.298	-1	13	5	19.651	19.545
-7	-3	4	7.416	7.504	7	3	4	18.061	17.435	4	8	4	4.615	5.827	-3	13	5	17.951	17.825
-9	-3	4	19.892	19.678	5	3	4	14.650	14.963	5	9	4	6.251	4.796	-5	13	5	11.332	9.916
-11	-3	4	11.417	10.456	3	3	4	8.687	9.849	3	9	4	25.469	26.597	-7	13	5	4.594	3.115
-10	-2	4	6.069	2.473	1	3	4	39.136	38.596	1	9	4	12.684	14.203	-6	12	5	17.125	18.334
-8	-2	4	23.541	21.974	-1	3	4	29.648	28.973	-1	9	4	41.077	42.899	-4	12	5	5.738	7.577
-6	-2	4	40.170	40.824	-3	3	4	23.418	22.989	0	6	0	98.444	95.817	-2	12	5	21.901	22.754

SUENO, PREWITT, AND FARRELL - HIGH ALBITE - 750 DEG. C

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
0	12	5	7.310	10.817	-5	5	5	16.642	17.540	-3	-1	5	11.667	12.293	1	-7	5	10.213	8.170
2	12	5	2.873 *	2.255	-7	5	5	4.242	2.560	-5	-1	5	18.358	19.733	-1	-7	5	30.571	29.236
3	11	5	14.603	14.169	-9	5	5	34.373	35.342	-7	-1	5	21.067	20.565	-3	-7	5	21.456	21.108
1	11	5	14.663	13.729	-10	4	5	17.116	17.412	-9	-1	5	3.321 *	0.647	-5	-7	5	11.620	13.557
-1	11	5	13.989	14.848	-8	4	5	22.350	22.378	-11	-1	5	13.535	13.167	-7	-7	5	10.628	12.137
-3	11	5	12.603	14.105	-6	4	5	5.051	0.296	-10	-2	5	24.376	24.408	-9	-7	5	7.255	6.333
-5	11	5	7.709	8.625	-4	4	5	58.181	58.690	-8	-2	5	29.152	29.247	-10	-8	5	6.602	6.426
-7	11	5	12.667	14.370	-2	4	5	13.908	13.543	-6	-2	5	28.440	27.944	-8	-8	5	15.803	16.935
-8	10	5	9.637	9.107	0	4	5	33.445	34.278	0	6	0	98.173	95.817	-6	-8	5	38.382	37.734
0	6	0	98.435	95.817	2	4	5	30.440	30.936	-4	-2	5	45.836	47.175	-4	-8	5	21.371	17.620
-6	10	5	13.349	13.516	4	4	5	12.862	13.815	-2	-2	5	14.654	16.127	-2	-8	5	44.993	46.748
-4	10	5	19.723	19.245	5	3	5	23.240	23.505	0	-2	5	37.915	37.661	0	-8	5	12.129	12.015
-2	10	5	6.708	2.294	3	3	5	21.575	21.704	2	-2	5	19.367	19.190	2	-8	5	3.505	2.904
0	10	5	10.319	9.392	1	3	5	21.354	20.520	4	-2	5	2.098 *	1.318	4	-8	5	20.134	19.847
2	10	5	11.705	10.491	-1	3	5	59.643	60.188	6	-2	5	5.971	3.552	3	-9	5	5.806	0.921
3	9	5	18.629	18.324	-3	3	5	22.214	21.446	5	-3	5	24.778	24.667	1	-9	5	24.227	24.073
1	9	5	24.096	23.649	-5	3	5	55.218	54.917	3	-3	5	17.184	17.569	-1	-9	5	20.231	16.971
-1	9	5	4.259	7.124	-7	3	5	27.164	25.970	1	-3	5	9.531	8.804	-3	-9	5	41.094	41.057
-3	9	5	58.909	59.432	-9	3	5	10.840	9.596	-1	-3	5	74.678	75.744	0	6	0	98.389	95.817
-5	9	5	9.891	6.783	0	6	0	98.499	95.817	-3	-3	5	5.039	4.303	-5	-9	5	22.710	23.796
-7	9	5	7.967	8.100	-11	3	5	18.044	18.596	-5	-3	5	68.665	68.171	-7	-9	5	4.293	1.936
-9	9	5	29.338	29.342	-10	2	5	7.009	8.129	-7	-3	5	36.627	36.564	-9	-9	5	27.529	27.042
-10	8	5	10.569	10.284	-8	2	5	17.345	17.946	-9	-3	5	2.759	2.271	-8	-10	5	6.899	6.211
-8	8	5	20.337	21.217	-6	2	5	22.816	22.157	-11	-3	5	28.287	27.816	-6	-10	5	3.039 *	1.218
-6	8	5	32.682	32.198	-4	2	5	4.289	2.883	-10	-4	5	12.302	11.132	-4	-10	5	10.289	9.094
-4	8	5	6.306	4.931	-2	2	5	28.385	28.331	-8	-4	5	4.662	6.517	-2	-10	5	3.992 *	2.440
-2	8	5	38.119	37.740	0	2	5	22.367	21.266	-6	-4	5	25.155	25.135	0	-10	5	4.153 *	6.491
0	8	5	20.485	19.688	2	2	5	8.696	7.855	-4	-4	5	25.251	45.922	2	-10	5	2.454 *	0.953
2	8	5	5.039	6.292	4	2	5	14.760	14.678	-2	-4	5	30.004	30.311	4	-10	5	3.810	4.771
4	8	5	19.968	19.880	6	2	5	4.229	2.334	0	6	0	98.601	95.817	3	-11	5	2.873 *	2.077
0	6	0	98.490	95.817	5	1	5	23.265	22.245	0	-4	5	26.461	27.870	1	-11	5	16.243	17.106
5	7	5	6.573	4.929	3	1	5	8.293	1.766	2	-4	5	29.275	29.930	-1	-11	5	4.123 *	0.104
3	7	5	4.009 *	0.996	1	1	5	18.011	18.259	4	-4	5	18.320	18.131	-3	-11	5	19.155	20.400
1	7	5	13.345	14.654	-1	1	5	70.674	70.483	6	-4	5	14.061	13.967	-5	-11	5	6.052	7.096
-1	7	5	18.083	15.154	-3	1	5	29.775	29.477	5	-5	5	2.594	0.379	-7	-11	5	7.912	8.789
-3	7	5	2.182 *	1.143	-5	1	5	43.742	45.283	3	-5	5	12.323	12.599	-8	-12	5	2.814 *	3.149
-5	7	5	16.896	17.418	-7	1	5	29.550	28.424	1	-5	5	45.539	46.008	-6	-12	5	21.392	21.305
-7	7	5	11.133	10.065	-9	1	5	8.276	8.079	-1	-5	5	3.471 *	5.095	-4	-12	5	9.438	10.325
-9	7	5	5.662	7.369	-11	1	5	26.236	26.790	-3	-5	5	46.658	46.533	-2	-12	5	24.223	24.459
-10	6	5	19.718	19.560	-10	0	5	32.275	32.095	-5	-5	5	12.404	11.822	0	6	0	98.562	95.817
-8	6	5	16.218	15.906	0	6	0	98.499	95.817	-7	-5	5	7.128	4.800	0	-12	5	4.462 *	0.160
-6	6	5	56.986	56.384	-8	0	5	32.161	32.341	-9	-5	5	32.025	32.794	2	-12	5	4.679	3.969
-4	6	5	27.033	26.436	-6	0	5	32.194	32.469	-10	-6	5	15.752	15.849	1	-13	5	15.014	14.517
-2	6	5	54.926	55.181	-4	0	5	105.008	105.052	-8	-6	5	13.569	12.827	-1	-13	5	23.571	23.167
0	6	5	29.211	30.340	-2	0	5	16.629	16.660	-6	-6	5	29.724	30.478	-3	-13	5	5.437	8.164
2	6	5	6.869	5.697	0	0	5	43.560	44.634	-4	-6	5	41.602	39.953	-5	-13	5	4.344 *	3.230
4	6	5	25.495	25.783	2	0	5	41.111	40.023	-2	-6	5	23.727	25.205	-7	-13	5	14.875	15.553
5	5	5	6.429	5.411	4	0	5	7.336	6.536	0	-5	5	24.121	23.534	-6	-14	5	5.132	0.257
3	5	5	20.134	19.906	6	0	5	22.075	21.819	2	-6	5	12.167	12.138	-4	-14	5	10.696	12.280
1	5	5	39.428	39.116	5	-1	5	10.107	10.365	4	-6	5	12.675	13.310	-2	-14	5	2.945 *	1.973
-1	5	5	28.639	28.174	3	-1	5	4.128	3.888	0	6	0	98.622	95.817	0	-14	5	9.302	9.360
0	6	0	98.677	95.817	1	-1	5	9.128	8.414	5	-7	5	3.543	1.516	-1	-15	5	6.039	6.213
-3	5	5	62.740	62.796	-1	-1	5	41.420	41.296	3	-7	5	4.806	3.419	-3	-15	5	5.441	5.976

SUENO, PREWITT, AND PAPKIN - HIGH ALBITE - 750 DEG. C

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H	K	L	F(OBS)	F(CALC)	H	K	L	F(OBS)	F(CALC)
-4	6	8	10.628	8.945	-4	-4	9	5.034	2.151
-2	6	8	4.590 *	5.273	-2	-4	9	4.738 *	3.158
0	6	8	6.310	4.724	-3	-5	9	9.349	8.229
0	5	0	98.486	95.817	-5	-5	9	22.303	22.403
-1	7	8	3.373 *	0.975	-7	-5	9	12.781	13.094
-3	7	8	4.573 *	0.127	-6	-6	9	18.684	19.218
-5	7	8	4.437 *	1.583	-4	-6	9	17.858	16.901
-7	7	8	4.407 *	1.601	-2	-6	9	12.544	11.746
-6	8	8	4.666	3.089	-3	-7	9	13.188	11.259
-4	8	8	6.280	7.551	-5	-7	9	8.213	7.158
-2	8	8	4.606	2.922					
-3	9	8	8.183	7.407					
-5	9	8	9.573	7.008					
-6	6	9	10.764	9.842					
-4	6	9	18.066	18.251					
-3	5	9	7.963	7.539					
-5	5	9	18.494	17.444					
-7	5	9	5.268	0.050					
-6	4	9	19.218	19.584					
-4	4	9	11.052	10.212					
-2	4	9	6.874	5.368					
-1	3	9	13.502	14.440					
-3	3	9	19.591	20.256					
-5	3	9	18.824	19.115					
0	6	0	98.719	95.817					
-7	3	9	16.468	15.699					
-8	2	9	13.315	14.104					
-6	2	9	4.547 *	2.556					
-4	2	9	7.200	6.216					
-2	2	9	10.688	11.921					
-1	1	9	6.840	2.582					
-3	1	9	30.033	30.535					
-5	1	9	4.543 *	1.711					
-7	1	9	13.485	14.321					
-8	0	9	5.674	5.716					
-6	0	9	34.707	35.006					
-4	0	9	21.808	23.012					
-2	0	9	14.214	13.396					
-1	-1	9	3.000 *	1.932					
-3	-1	9	9.738	10.035					
-5	-1	9	4.543 *	0.005					
-7	-1	9	6.208	4.943					
-8	-2	9	10.628	9.113					
-6	-2	9	23.316	23.930					
-4	-2	9	17.947	18.747					
0	6	0	98.575	95.817					
-2	-2	9	13.353	13.501					
-1	-3	9	5.242	4.161					
-3	-3	9	35.576	36.070					
-5	-3	9	11.184	13.874					
-7	-3	9	19.964	19.772					
-8	-4	9	12.527	13.967					
-6	-4	9	9.972	10.907					

ATOM	PARAMETER	OLD	CHANGE	NEW	ERROR	SHIFT/ERROR
	EXTINCTION CORRECTION	0.0		0.0		
	SCALE FACTOR 1	2.3597	0.0002	2.3599	0.00576	0.03
ATOM 1	NAI EQUIPOINT FRACTION = 1.000					
	OCCUPANCY SPECIES 1	1.00000		1.00000		
	X	0.2767949	0.0000605	0.2768553	0.0004594	0.13
	Y	0.0028003	0.000493	0.0028506	0.0004202	0.12
	Z	0.1375150	-0.0001438	0.1373711	0.0007098	-0.20
	BETA11	0.0183713	0.0000243	0.0163956	0.0006622	0.04
	BETA22	0.0241686	0.0001239	0.0242925	0.0006020	0.21
	BETA33	0.0624428	-0.0000710	0.0623718	0.0016311	-0.04
	BETA12	0.0007629	0.0001419	0.0009047	0.0004899	0.29
	BETA13	0.0090822	0.0000207	0.0091029	0.0008360	0.02
	BETA23	-0.0135906	0.0002013	-0.0133093	0.0007870	0.26
ATOM 2	T10 EQUIPOINT FRACTION = 1.000			0.75000		
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.0087405	-0.0000051	0.0087354	0.0001459	-0.04
	Y	0.1718670	-0.0000184	0.1718407	0.0000841	-0.22
	Z	0.2188423	0.0000250	0.2188673	0.0001644	0.15
	BETA11	0.0091685	0.0000039	0.0091724	0.0001807	0.02
	BETA22	0.0030955	0.0001494	0.0031103	0.0000597	0.25
	BETA33	0.0101944	0.0000914	0.0102058	0.0002323	0.39
	BETA12	-0.0007101	0.0000296	-0.0006804	0.0000804	0.37
	BETA13	0.0046976	0.0000447	0.0047422	0.0001672	0.27
	BETA23	0.00001996	0.0000414	0.00002410	0.0000913	0.45
ATOM 3	TIM EQUIPOINT FRACTION = 1.000			0.75000		
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.0066175	0.0000186	0.0066361	0.0001446	0.13
	Y	0.8176479	0.0000245	0.8176724	0.0000840	0.29
	Z	0.2267377	0.0000207	0.2267502	0.0001623	0.13
	BETA11	0.0090867	-0.0000145	0.0090723	0.0001807	-0.08
	BETA22	0.0031045	0.0000074	0.0031120	0.0000595	0.13
	BETA33	0.0097799	-0.0001153	0.0096646	0.0002292	-0.50
	BETA12	0.0011330	-0.0000345	0.0010985	0.0000803	-0.43
	BETA13	0.0045957	-0.0000473	0.0045484	0.0001669	-0.28
	BETA23	0.0006774	-0.0000513	0.0006261	0.0000910	-0.56
ATOM 4	T20 EQUIPOINT FRACTION = 1.000			0.75000		
	OCCUPANCY SPECIES 2	0.75000		0.75000		
	OCCUPANCY SPECIES 4	0.25000		0.25000		
	TOTAL OCCUPANCY (FIXED) =	1.00000				
	X	0.6939956	0.0000248	0.6940204	0.0001427	0.17
	Y	0.1122922	0.0000290	0.1123213	0.0000809	0.36
	Z	0.3315108	0.0000686	0.3315794	0.0001728	0.40
	BETA11	0.0081650	-0.0000104	0.0081546	0.0001745	-0.06
	BETA22	0.0024767	-0.0000057	0.0024710	0.0000555	-0.10
	BETA33	0.0130523	-0.0000665	0.0129858	0.0002514	-0.26
	BETA12	-0.0002196	-0.0000258	-0.0002454	0.0000761	-0.34
	BETA13	0.0041245	-0.0000392	0.0040853	0.0001700	-0.23
	BETA23	0.0003220	-0.0000380	0.0002841	0.0000917	-0.41