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Crystal structure refinement of lawsonite

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Abstract

Lawsonite, $Ca^{6}Al_2^{6}Si_2^{4}O_7(OH)_2 \cdot H_2O$, is found in low-temperature, high-pressure metamorphic rocks. It is a hydrous counterpart of anorthite. A specimen from the type locality, Tiburon Peninsula, Marin County, California, was used for an X-ray study: $a = 8.795(3)$, $b = 5.847(1)$, $c = 13.142(6)$Å, $V = 675.8$Å, $Z = 4$, $D_{calc} = 3.088$ g.cm^{-3}, space group *Ccmm*. Refinement of 865 F_{obs} gave an $R = 0.0256$. The structure is based on a three dimensional framework generated by cross-linking ribbons composed of edge sharing single chains of Al coordination octahedra and lateral bridging silicate groups. The openings of the framework accommodate the Ca atoms and the water molecules. The observed mean distances are $Si^{4} - O = 1.633$, $Al^{6} - O = 1.913$ and $Ca^{8} - O = 2.421$Å. The hydrogen atoms participate in bent and bifurcated hydrogen bonds. Individual cation-anion distances conform well to the extended electrostatic valence rule.

Introduction

The crystal structure of lawsonite, $CaAl_2Si_2O_7(OH)_2 \cdot H_2O$, was determined by Wickman (1947) in space group $C222_1$. The Si–O bond lengths in the Si_2O_7 group as found by Wickman ranged from 1.59 to 1.72 Å. Subsequently, the structure was refined by Rumanova and Skipetrova (1959). They found that it could be described in the centric space group *Ccmm* and that the Si–O distances were lying in a narrow range: between 1.65 and 1.69Å. Recently Pabst (1977) pointed out that lawsonite is denser than anorthite, its anhydrous equivalent. The volume per oxygen atom in lawsonite is 18.74Å, while in anorthite it is 20.94A. Lawsonite is one of several especially dense hydrous silicates found in the Franciscan Formation, California. It is typical of a low-temperature, high-pressure metamorphic paragenesis.

Experimental

A clear, almost colorless specimen of lawsonite from the type locality, Tiburon Peninsula, Marin County, California (USNM R3922) was divided into two parts: one was ground into a sphere with a diameter of 0.04 cm, the other was used for a microprobe analysis. Data were collected on an automatic four-circle diffractometer ($\lambda AgK\alpha = 0.56083$Å), using procedures described by Baur and Khan (1970). The unit cell constants were refined from the setting of 20 reflections measured on a single crystal X-ray diffractometer. The resulting cell constants agree closely with those reported by Davis and Pabst (1960). Reciprocal space was searched in a sphere of radius $\sin\theta/\lambda = 0.84$Å^{-1}. The total number of measured reflections was 11,268, which were averaged to yield 1,928 unique reflections. Of these 1,063 had an intensity of less than two sigma, and were not used in the refinement. The systematic absences (*hkl* only present with $h + k = 2n$; and 0*kl* only with $l = 2n$) are consistent with space group *Ccmm* as noted by Rumanova and Skipetrova. The successful refinement confirms this choice. Lorentz-polarization corrections were applied, but because of the small linear absorption coefficient and the size of the crystal, an absorption correction was not necessary. Scattering factors were taken from the *International Tables for X-ray Crystallography (1974)*. The refinement of the 865 observed unique structure factors started with the parameters reported by Rumanova and Skipetrova (1959) and refined in a few cycles to an $R\ (=\Sigma||Fo| - |Fc||/\Sigma|Fo|)$ of 0.027 (with anisotropic temperature factors). A difference synthesis revealed likely positions for the hydrogen atoms. Upon further refinement including the hydrogen atoms an R of 0.0256 was achieved. The positional (Table 1) and the thermal (Table 2) parameters were used to

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LAWSONITE, ANISOTROPIC, WITH H-ATOMS
PRE-CYCLE 1

H	K	L	Y(OBS)	Y(CALC)
0	0	2	28.7310	27.3214
0	0	4	12.3837	13.1257
0	0	6	35.2238	33.6005
0	0	8	90.6994	94.6195
0	0	10	22.0231	22.4152
0	0	12	5.5646	5.8401
0	0	14	4.9943	4.9474
0	0	16	55.9445	54.7331
0	0	20	13.6539	12.7320
0	2	0	65.1444	61.1066
0	2	2	64.3958	60.8620
0	2	4	21.8407	20.6073
0	2	6	63.7288	65.8544
0	2	8	13.3353	13.6832
0	2	10	78.4209	85.0241
0	2	12	9.2757	9.5048
0	2	14	11.2725	11.7503
0	2	16	11.3257	11.4768
0	2	18	35.8347	35.7494
0	2	20	2.9617	2.2269
0	4	0	136.1954	138.3727
0	4	2	16.7393	16.1480
0	4	4	12.6873	11.4382
0	4	6	8.9800	8.5985
0	4	8	61.2595	64.0050
0	4	10	14.9548	15.5144
0	4	12	5.5468	5.7234
0	4	14	5.4559	5.2095
0	4	16	42.9871	43.2243
0	4	20	11.3807	11.1425
0	6	0	26.0930	26.1045
0	6	2	30.0875	30.0396
0	6	4	9.9012	9.7643
0	6	6	32.2455	32.3449
0	6	8	2.1666	1.5848
0	6	10	47.1452	47.9973
0	6	12	9.1682	8.9909
0	6	14	8.1531	8.2747
0	6	16	9.9796	9.5506
0	8	0	54.8151	55.3110
0	8	2	7.2477	7.2208
0	8	4	8.0151	8.2432
0	8	6	2.5414	2.3206
0	8	8	28.7914	28.8812
0	8	10	10.2728	10.1417
0	8	12	4.9011	5.1434
1	1	0	38.9341	31.3236
1	1	1	18.5686	15.5581
1	1	2	6.9562	6.9206
1	1	3	27.1428	26.4927
1	1	4	60.0037	60.3869
1	1	5	23.9158	23.8595
1	1	6	12.1416	12.7745
1	1	7	19.3140	20.1786
1	1	8	18.5092	19.6269
1	1	9	1.8973	2.0608
1	1	10	1.7139	2.2092
1	1	11	19.5786	20.3293
1	1	12	19.5446	20.5246
1	1	13	11.6091	12.1001
1	1	14	21.4830	21.9912
1	1	15	3.4388	4.2233
1	1	16	10.5026	10.5956
1	1	17	11.0024	11.0531
1	1	18	6.1099	6.0284
1	1	20	12.2594	11.8265
1	1	21	8.7061	8.4148
1	3	0	12.5086	12.1125
1	3	1	25.0742	22.8098
1	3	2	3.4985	3.8292
1	3	3	10.5054	10.6191
1	3	4	34.6493	34.7379
1	3	5	13.9949	13.9310
1	3	6	13.9704	13.8448
1	3	7	23.5844	23.9684
1	3	8	9.2463	9.8879
1	3	9	5.1709	5.2222
1	3	10	5.2014	5.6068
1	3	11	11.6056	12.0628
1	3	12	13.0875	13.4948
1	3	13	9.8704	10.1970
1	3	14	21.7184	22.2954
1	3	15	8.0267	8.1633
1	3	16	7.1119	6.8539
1	3	17	10.5280	10.4940
1	3	18	8.1892	7.9513
1	3	20	9.5706	9.1161
1	5	0	27.8573	28.0319
1	5	1	5.8743	5.5367
1	5	2	3.6457	3.6413
1	5	3	20.1011	20.0269
1	5	4	39.4019	39.7629
1	5	5	17.7751	17.9876
1	5	6	7.0908	6.9343
1	5	7	7.3010	7.2951
1	5	8	18.2722	18.7020
1	5	11	18.1400	18.5470
1	5	12	17.5346	17.8596
1	5	13	10.1885	10.1546
1	5	14	13.7053	13.6658
1	5	16	10.3949	10.3604
1	5	17	9.4356	9.2343
1	5	18	3.0238	2.6721
1	7	0	6.2379	6.3779
1	7	1	13.3204	13.4278
1	7	2	1.6780	1.2949
1	7	3	4.6803	4.4857
1	7	4	15.3810	15.2835
1	7	5	7.2564	7.2525
1	7	6	8.3448	8.3979
1	7	7	15.6920	15.7620
1	7	8	3.2087	3.2783
1	7	9	5.0661	5.1414
1	7	10	4.6845	4.7510
1	7	11	5.5858	5.6957
1	7	12	5.6687	5.5850
1	7	13	6.8825	6.7522
1	7	14	15.5423	15.3813
1	7	15	8.3157	8.1207
1	9	0	15.0682	15.0764
1	9	1	2.8263	2.7521
1	9	2	2.2996	2.0443
1	9	3	11.9209	11.9859
1	9	4	20.8824	20.8324
1	9	5	10.7043	10.8137
1	9	6	3.0085	2.7002
1	9	7	2.8060	3.0831
1	9	8	10.9567	10.7864
2	0	0	8.1304	7.4850
2	0	1	33.8683	28.6040
2	0	2	48.9819	46.7373
2	0	3	3.0083	3.2693
2	0	4	77.2870	77.3035
2	0	5	60.5911	60.0901
2	0	6	17.9046	17.4271
2	0	7	54.8374	56.8957
2	0	9	21.5927	22.3270
2	0	10	28.5276	30.3297
2	0	11	21.3678	23.1773
2	0	12	39.4029	41.0162
2	0	13	8.1470	9.1201
2	0	14	3.5177	3.5159
2	0	15	10.5219	10.6613
2	0	16	5.9863	6.0938
2	0	17	7.5733	7.7829
2	0	18	19.8484	19.3179
2	0	20	17.2986	16.3120
2	2	0	64.2540	58.7858
2	2	1	33.8967	30.4461
2	2	2	31.7315	29.4426
2	2	3	69.2844	66.3710
2	2	4	1.8898	2.1028
2	2	5	14.6172	14.1735
2	2	6	43.5427	45.0738
2	2	7	2.7347	2.4962
2	2	8	47.5565	50.4102
2	2	9	7.3338	7.9550
2	2	10	15.4308	15.9446
2	2	11	10.5654	10.9276
2	2	13	12.0676	12.1379
2	2	14	28.9680	29.7188
2	2	15	10.8153	11.1832
2	2	16	19.5786	19.7042
2	2	17	8.9742	9.1967
2	2	19	14.0986	13.5757
2	2	21	3.2918	3.4436
2	4	0	6.2406	6.2522
2	4	1	18.4547	18.3354
2	4	2	28.9921	28.5621
2	4	3	8.6995	8.0772
2	4	4	56.0509	56.6706
2	4	5	25.1667	25.7640
2	4	6	11.5635	11.5413
2	4	7	32.6380	33.7804
2	4	8	1.4358	0.7423
2	4	9	16.3494	16.6288
2	4	10	22.1906	22.7069
2	4	11	12.6318	13.0221

2	4	12	31.7849	32.6768	3	3	6	11.7304	11.7744	4	0	10	25.3602	26.0793
2	4	13	8.5360	8.6651	3	3	7	5.1566	4.8172	4	0	11	18.1694	18.5170
2	4	14	2.3939	2.0740	3	3	8	46.2373	48.2819	4	0	12	11.1264	11.3876
2	4	15	8.1642	8.1507	3	3	9	9.5948	9.9581	4	0	13	26.1212	26.6763
2	4	16	5.1743	5.1693	3	3	10	26.6044	27.9499	4	0	14	37.3777	38.0127
2	4	17	7.2813	6.9827	3	3	12	8.3622	8.5370	4	0	15	9.5808	9.7149
2	4	18	16.0460	15.7016	3	3	13	5.0738	5.1351	4	0	16	4.0688	3.9144
2	6	0	33.4474	32.9579	3	3	14	10.7714	11.2480	4	0	17	5.3783	5.1392
2	6	2	18.8354	18.5986	3	3	16	19.0087	18.8533	4	0	18	3.7675	3.6777
2	6	3	24.3167	24.1116	3	3	18	16.8118	16.3656	4	0	19	10.3749	10.1212
2	6	4	4.5295	3.9510	3	3	19	5.5952	5.3560	4	0	21	11.1883	10.6401
2	6	5	5.3270	5.2316	3	3	20	6.2545	5.9505	4	2	0	19.3717	19.0956
2	6	6	26.7054	27.0410	3	5	0	33.5288	33.5655	4	2	1	17.8020	16.4581
2	6	7	7.8296	7.9345	3	5	1	10.6848	10.9074	4	2	2	39.5546	37.5719
2	6	8	28.5143	29.0707	3	5	2	20.6578	20.2603	4	2	3	42.3699	42.5527
2	6	9	8.7499	8.6996	3	5	3	11.2441	11.2664	4	2	4	96.3848	99.3229
2	6	10	10.0746	10.2529	3	5	4	6.7117	6.8104	4	2	5	28.2498	28.5063
2	6	11	5.5699	5.5877	3	5	5	10.9412	11.3187	4	2	6	3.1052	2.8666
2	6	13	8.9733	8.9975	3	5	6	5.0561	5.0897	4	2	7	21.9870	22.3366
2	6	14	19.9791	19.9896	3	5	7	6.3701	6.6597	4	2	8	18.9948	20.1806
2	6	15	4.7107	4.6448	3	5	8	27.0994	27.8461	4	2	9	8.6379	8.9019
2	6	16	12.8731	12.7007	3	5	9	10.5049	10.7241	4	2	10	2.3195	2.0623
2	6	17	7.8893	7.5574	3	5	10	24.7968	25.5025	4	2	11	13.4950	14.0556
2	8	0	2.9128	3.0615	3	5	11	9.5043	9.6355	4	2	12	44.1197	45.7041
2	8	1	8.0737	8.1397	3	5	13	5.7721	5.7209	4	2	13	25.4785	25.9177
2	8	2	12.1443	12.2350	3	5	14	5.3500	5.6178	4	2	14	7.5173	7.6058
2	8	3	9.2397	9.2549	3	5	15	5.1243	5.2073	4	2	15	10.9361	10.9460
2	8	4	28.5494	28.8639	3	5	16	11.6217	11.2693	4	2	16	7.3818	7.7271
2	8	5	7.7814	7.6622	3	5	18	17.9319	17.1775	4	2	17	4.3869	4.1859
2	8	6	4.1399	4.3199	3	7	0	34.9406	35.2703	4	2	18	11.4415	10.9577
2	8	7	15.7424	15.6288	3	7	1	1.6085	1.5071	4	2	19	8.7179	8.2804
2	8	9	9.3058	9.2313	3	7	2	13.2247	13.2425	4	2	20	22.8356	21.5591
2	8	10	11.2211	11.0936	3	7	3	1.9693	1.8882	4	4	1	8.4025	7.3436
2	8	11	3.5238	3.4944	3	7	4	6.9169	6.6696	4	4	2	16.1962	15.9305
2	8	12	18.6533	18.5322	3	7	5	2.2380	2.2309	4	4	3	33.0742	33.9473
3	1	0	76.9769	73.2220	3	7	6	6.7054	6.7151	4	4	4	5.1811	4.9046
3	1	1	14.2665	13.8756	3	7	7	5.7713	5.6704	4	4	5	23.5675	23.2425
3	1	2	43.9367	41.0333	3	7	8	29.3949	29.6101	4	4	6	47.9113	48.5764
3	1	3	9.7826	8.9729	3	7	9	4.2057	4.1786	4	4	7	13.4092	13.6550
3	1	4	14.9323	14.0969	3	7	10	15.0800	15.2941	4	4	8	29.1509	29.7340
3	1	5	11.2608	10.6368	3	7	12	7.0110	7.0821	4	4	9	6.2857	6.2289
3	1	6	12.5554	12.9149	3	7	13	3.2571	3.1618	4	4	10	19.5625	19.8597
3	1	7	3.5656	3.2470	3	7	14	8.9694	9.1238	4	4	11	14.0259	14.1782
3	1	8	46.9881	49.3035	3	9	0	14.0962	14.4032	4	4	12	7.2637	7.2824
3	1	9	14.4981	14.8946	3	9	1	6.0649	5.9837	4	4	13	21.1089	21.4078
3	1	10	33.3351	35.4968	3	9	2	10.0872	10.1822	4	4	14	29.1725	29.3692
3	1	11	7.0254	7.3707	3	9	3	7.3956	7.4370	4	4	15	7.3708	7.9413
3	1	12	4.6568	4.6878	3	9	4	5.3607	5.4951	4	4	16	4.1664	3.9970
3	1	13	6.3326	6.4089	3	9	5	7.2383	7.0827	4	4	17	4.4483	4.3312
3	1	14	9.5003	9.9193	3	9	6	2.2462	2.2219	4	4	18	3.3133	2.8993
3	1	15	2.8490	3.2120	3	9	7	4.8666	4.7745	4	4	19	9.1197	8.5729
3	1	16	18.0535	18.0253	4	0	0	36.5361	33.6137	4	6	0	11.0645	11.2851
3	1	18	20.6403	20.2423	4	0	1	16.4872	15.8072	4	6	1	6.6625	6.3118
3	1	20	8.4954	8.1913	4	0	2	17.5669	17.5103	4	6	2	21.0909	21.1464
3	1	21	5.2648	4.7298	4	0	3	56.1802	55.3217	4	6	3	21.4901	21.7157
3	3	0	68.7821	66.9670	4	0	4	16.2770	14.5998	4	6	4	48.5718	48.9942
3	3	1	2.2898	1.7680	4	0	5	33.8307	33.8926	4	6	5	16.3629	16.1487
3	3	2	30.3503	28.7600	4	0	6	69.5118	72.0142	4	6	6	2.0579	1.8764
3	3	3	1.9642	1.2148	4	0	7	20.7708	21.1326	4	6	7	11.9087	11.9477
3	3	4	3.6488	3.5817	4	0	8	32.6222	34.3015	4	6	8	8.8690	8.7959
3	3	5	4.4277	4.7958	4	0	9	8.7471	9.7047	4	6	9	5.1040	5.0793

(3)

4	6	10	3.0636	2.9900	5	5	3	3.7675	3.5298	6	2	10	2.4824	2.4133
4	6	11	9.0099	9.0550	5	5	4	13.1205	12.9680	6	2	11	8.8804	9.0795
4	6	12	27.0244	27.0107	5	5	6	11.9529	12.0865	6	2	12	10.2690	10.4712
4	6	13	17.4226	17.4395	5	5	7	9.5537	9.5563	6	2	13	19.4951	19.6343
4	6	14	4.5125	4.3846	5	5	8	5.2362	4.9438	6	2	14	12.1010	12.3148
4	6	15	7.7596	7.5805	5	5	9	8.3818	8.3745	6	2	15	12.6885	12.6248
4	6	16	6.9028	6.6956	5	5	10	5.6123	5.6702	6	2	16	27.2337	26.6550
4	8	0	6.1621	6.1342	5	5	11	11.5190	11.4442	6	2	17	6.1683	6.0819
4	8	1	3.4939	3.4867	5	5	12	10.5605	10.5149	6	2	19	8.1783	7.7329
4	8	2	7.7659	7.7445	5	5	13	2.2548	2.5048	6	4	0	13.0663	13.0560
4	8	3	16.8306	16.9792	5	5	14	9.8133	9.8242	6	4	1	6.2176	6.4919
4	8	4	2.0458	1.7312	5	5	15	2.0550	1.75[illegible]3	6	4	2	28.6047	28.0509
4	8	5	12.2084	12.0639	5	5	17	14.5324	13.8789	6	4	3	11.5111	11.5182
4	8	6	23.5927	23.8699	5	7	0	15.4776	15.3451	6	4	4	22.1761	22.0424
4	8	7	7.3230	7.4916	5	7	1	17.2624	17.0716	6	4	5	5.1034	4.9651
4	8	8	19.1521	19.1591	5	7	2	3.5627	3.5614	6	4	6	26.5491	26.8358
4	8	9	3.6558	3.6766	5	7	3	4.9099	4.6772	6	4	7	12.1988	12.1812
4	8	10	12.2007	12.0806	5	7	4	21.1994	21.3119	6	4	8	1.9681	1.5294
4	8	11	8.1841	8.0580	5	7	5	4.8887	4.8176	6	4	9	6.4608	6.6733
5	1	0	18.2612	18.9426	5	7	6	6.5965	6.5565	6	4	10	33.9815	34.7715
5	1	1	22.2382	21.3165	5	7	7	15.9592	15.8395	6	4	11	10.5830	10.7095
5	1	2	1.6583	1.4888	5	7	8	12.6874	12.5526	6	4	12	14.6296	14.5634
5	1	3	3.2680	2.3844	5	7	9	9.9937	9.7434	6	4	13	15.4807	15.4838
5	1	4	23.0253	23.1335	5	7	11	2.1640	2.1229	6	4	14	9.3334	9.5224
5	1	5	5.9012	6.0293	5	7	12	15.4039	15.3853	6	4	15	3.5752	3.3510
5	1	6	13.3879	13.8195	5	7	13	3.3235	3.1064	6	4	16	4.5939	4.2579
5	1	7	17.7409	18.2077	5	9	1	6.3928	6.4215	6	4	17	6.0262	5.9398
5	1	8	14.0894	14.8257	5	9	2	2.0150	1.7372	6	6	0	44.4392	45.0195
5	1	9	12.0133	11.9659	5	9	3	4.2163	4.1086	6	6	1	16.2222	16.2340
5	1	10	6.4669	6.8194	5	9	4	5.0987	5.3126	6	6	2	9.3407	9.3239
5	1	11	10.2883	10.2743	6	0	0	18.2787	17.0551	6	6	3	22.8721	22.7566
5	1	12	17.0564	17.2962	6	0	1	6.6504	5.[illegible]504	6	6	4	10.4830	10.7477
5	1	13	5.1478	5.3687	6	0	2	36.3562	35.4318	6	6	5	4.7202	4.6084
5	1	14	9.5103	9.5239	6	0	3	11.4582	11.4653	6	6	6	5.4273	5.2467
5	1	16	2.6614	2.7684	6	0	4	28.0465	29.1527	6	6	7	4.0709	4.0529
5	1	17	17.9677	17.3698	6	0	5	11.9016	12.3624	6	6	8	27.1658	27.1987
5	1	18	6.4513	6.2300	6	0	6	33.6320	34.4130	6	6	9	9.0361	9.1170
5	1	20	4.8435	4.4885	6	0	7	19.0479	19.7805	6	6	10	3.2611	3.3057
5	3	0	25.4837	25.1786	6	0	8	4.6059	4.0399	6	6	11	4.3337	4.0929
5	3	1	25.2576	24.9859	6	0	9	7.3266	7.6185	6	6	12	7.5690	7.7285
5	3	2	3.4390	3.1283	6	0	10	41.[illegible]906	43.1918	6	6	13	13.8936	13.5579
5	3	3	7.4195	7.5624	6	0	11	15.6228	15.8685	6	6	14	7.6658	7.5733
5	3	4	29.9950	29.8323	6	0	12	18.8894	19.3060	6	8	0	8.6674	8.9064
5	3	5	8.1653	8.7087	6	0	13	17.8382	18.0784	6	8	1	5.2550	5.4281
5	3	6	10.5711	10.5621	6	0	14	10.9639	11.0698	6	8	2	15.5132	15.6529
5	3	7	21.0275	21.6535	6	0	15	5.1440	5.0475	6	8	3	9.6353	9.5964
5	3	8	18.5666	18.7233	6	0	16	4.8761	4.4536	6	8	4	9.9610	10.0196
5	3	9	13.3472	13.4123	6	0	17	7.5437	7.3698	6	8	6	15.5637	15.7661
5	3	10	2.8759	2.7307	6	0	18	21.6092	20.7514	6	8	7	5.0951	4.9409
5	3	11	5.1656	5.1001	6	0	19	5.9062	5.8320	7	1	0	7.5327	7.6827
5	3	12	19.4252	19.8743	6	0	20	5.4653	5.3898	7	1	1	9.1607	9.1441
5	3	13	5.1400	5.4473	6	2	0	74.4636	74.3945	7	1	2	8.5461	8.5222
5	3	14	6.2102	6.3700	6	2	1	34.4642	34.4445	7	1	3	33.2194	32.9681
5	3	15	4.1732	4.2101	6	2	2	19.2256	19.1236	7	1	4	31.7202	32.4354
5	3	16	4.8215	4.7499	6	2	3	44.2445	44.2559	7	1	5	34.1085	35.2113
5	3	17	16.9015	16.2944	6	2	4	16.9342	16.3128	7	1	6	9.3058	9.2978
5	3	18	3.3845	2.9933	6	2	5	9.0762	8.7318	7	1	7	12.2873	12.3490
5	3	19	2.1392	2.2915	6	2	6	11.0797	10.8133	7	1	8	3.3541	3.4495
5	5	0	6.0891	5.4388	6	2	7	11.3396	11.6655	7	1	9	3.9347	3.9724
5	5	1	12.8416	12.7292	6	2	8	39.8770	41.0631	7	1	10	4.7797	4.6257
5	5	2	2.4221	1.9153	6	2	9	16.2186	16.6010	7	1	11	14.9496	15.2772

7	1	12	11.1041	11.1019
7	1	13	25.3883	25.5103
7	1	14	18.0451	18.1374
7	1	15	12.3960	12.2931
7	1	16	4.3959	4.3566
7	1	19	8.5393	8.1047
7	3	0	1.5714	1.1261
7	3	1	2.2322	1.7342
7	3	2	6.4871	6.5250
7	3	3	33.3159	33.4366
7	3	4	22.6603	22.6689
7	3	5	32.8733	33.4880
7	3	6	9.2762	9.3411
7	3	7	5.3400	5.1253
7	3	8	1.9240	1.3897
7	3	10	2.7493	2.4077
7	3	11	17.5767	17.9735
7	3	12	6.3842	6.8912
7	3	13	23.5507	23.4367
7	3	14	18.2079	18.2313
7	3	15	7.3593	7.6091
7	3	16	2.0704	1.7299
7	3	18	2.3620	1.9652
7	5	0	10.5033	10.1351
7	5	1	7.6080	7.5525
7	5	2	5.9880	5.9483
7	5	3	17.5856	17.6004
7	5	4	25.9583	25.7524
7	5	5	21.1395	21.2770
7	5	6	5.8904	5.8362
7	5	7	11.5827	11.8201
7	5	8	5.5930	5.6517
7	5	9	3.7026	3.6900
7	5	10	4.8134	4.8139
7	5	11	7.2180	7.3285
7	5	12	10.8309	10.5413
7	5	13	18.6759	18.4514
7	5	14	12.3020	12.7364
7	5	15	12.1170	12.0666
7	7	1	1.8027	1.7948
7	7	2	3.4636	3.5735
7	7	3	21.3650	21.5557
7	7	4	11.0773	11.1325
7	7	5	20.6975	20.8694
7	7	6	6.1393	6.1186
7	7	8	3.4859	3.4495
7	7	11	13.5917	13.6475
8	0	0	58.5083	59.5759
8	0	1	21.1763	21.3876
8	0	2	40.4333	40.8362
8	0	3	12.5550	12.4044
8	0	4	12.5374	12.7747
8	0	5	12.3033	12.8601
8	0	6	20.0890	20.1821
8	0	7	19.7772	20.1427
8	0	8	23.3275	23.8936
8	0	9	24.5479	25.2950
8	0	10	14.4898	15.0581
8	0	11	3.4412	3.1845
8	0	12	10.3555	10.3034
8	0	14	17.2806	16.8756
8	0	15	2.3656	2.6793
8	0	16	18.6655	18.3891
8	0	17	16.1834	15.8531
8	0	18	16.4130	15.7541
8	2	0	18.1803	17.8191
8	2	1	23.7879	23.9750
8	2	2	6.2835	6.1475
8	2	3	6.6010	6.3934
8	2	4	23.0753	23.1780
8	2	5	14.2473	14.3645
8	2	6	9.3667	9.6110
8	2	7	23.7929	24.0919
8	2	8	32.0222	32.8955
8	2	9	23.3584	23.9626
8	2	10	24.8503	25.2419
8	2	11	1.7353	0.7941
8	2	12	19.9763	19.8346
8	2	14	5.1614	5.1734
8	2	15	6.3558	5.9186
8	2	16	10.9806	10.9948
8	2	17	13.5767	13.3546
8	4	0	42.4211	42.3610
8	4	1	16.9696	16.9316
8	4	2	31.4579	31.5426
8	4	3	9.0736	9.0510
8	4	4	8.5937	8.5086
8	4	5	9.9705	10.1592
8	4	6	16.7639	16.8695
8	4	7	16.0735	16.0770
8	4	8	17.0209	16.7982
8	4	9	20.1778	20.3565
8	4	10	11.6660	11.8007
8	4	11	2.8908	2.5216
8	4	12	8.2145	8.0746
8	4	14	14.9204	14.8357
8	4	15	1.9941	2.0852
8	4	16	15.1453	14.5382
8	6	0	8.6415	8.5877
8	6	1	15.6650	15.4671
8	6	2	3.2138	2.4818
8	6	3	4.3414	4.2907
8	6	4	18.1438	18.2889
8	6	5	9.1920	9.4242
8	6	6	6.0606	5.9556
8	6	7	16.2994	16.1254
8	6	8	20.3684	20.5570
8	6	9	16.4361	16.2606
8	6	10	15.8538	15.7728
8	6	12	15.7427	15.8040
8	8	0	20.1802	20.2087
8	8	1	9.6451	9.4424
8	8	2	18.0926	18.3290
8	8	3	5.9847	5.8623
8	8	4	3.1933	3.0216
9	0	16	1.8689	3.4459
9	1	0	18.2440	17.7788
9	1	1	13.1018	13.1705
9	1	2	6.4377	6.3912
9	1	3	12.1779	11.9563
9	1	4	4.8132	4.7374
9	1	5	16.3778	16.6502
9	1	6	4.0209	3.9418
9	1	7	3.1390	3.2652
9	1	8	12.6000	12.9704
9	1	9	18.4397	18.9613
9	1	10	8.3011	8.3380
9	1	11	9.1963	9.2263
9	1	13	11.8501	11.7107
9	1	15	3.2779	3.2875
9	1	16	8.3074	7.8928
9	1	17	3.1387	2.8319
9	3	0	11.5251	11.1140
9	3	1	8.6559	8.8004
9	3	2	6.7914	6.8015
9	3	3	7.5164	7.2306
9	3	4	1.8472	1.7235
9	3	5	12.4917	12.6056
9	3	6	2.7257	2.5270
9	3	8	7.9978	8.1080
9	3	9	15.2929	15.6725
9	3	10	9.9858	9.9070
9	3	11	5.4706	5.4273
9	3	12	2.3432	2.0629
9	3	13	9.9630	9.8156
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9	5	0	18.4872	18.4086
9	5	1	11.5773	11.7484
9	5	2	5.7900	5.7871
9	5	3	11.3389	10.9576
9	5	4	6.0910	6.0783
9	5	5	13.9208	13.6931
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9	5	7	4.7654	4.9632
9	5	8	13.9018	13.9895
9	5	9	15.2668	15.5213
9	5	10	5.6737	5.6821
9	5	11	9.6544	9.4782
9	5	12	3.3171	2.9896
9	5	13	9.6747	9.3104
9	7	0	5.1689	5.2565
9	7	1	3.5872	3.8063
9	7	2	5.9128	5.8501
9	7	3	2.8029	2.4196
9	7	4	5.5298	5.5653
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9	7	6	2.0409	1.9513
9	7	7	2.6488	2.0657
10	0	0	24.3529	24.3715
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10	0	2	18.1912	18.1759
10	0	3	23.9534	24.0148
10	0	4	32.5120	32.4810
10	0	5	38.5800	39.2088
10	0	6	3.8976	4.0628
10	0	7	10.7342	10.7652
10	0	8	4.9319	5.1682
10	0	9	7.5114	7.5173
10	0	10	2.2579	2.1666
10	0	11	23.3549	23.4904
10	0	12	18.6254	18.3736
10	0	13	16.3734	16.1197
10	0	14	6.1604	5.9018

10	0	15	2.2505	2.0431	11	3	9	18.6470	18.5392	13	3	4	6.3102	6.1914
10	0	16	12.5617	12.1542	11	3	10	4.0992	4.2384	13	3	5	14.3433	14.6629
10	2	0	3.6993	3.6075	11	3	11	7.7284	7.8475	13	3	6	2.4505	2.1339
10	2	1	8.5134	8.4496	11	3	12	13.3425	13.1856	13	3	7	4.4305	4.2232
10	2	2	13.9116	14.0670	11	5	0	6.9109	7.0774	14	0	0	11.6024	11.5250
10	2	3	4.8233	4.9199	11	5	1	20.3656	20.4268	14	0	1	12.7986	12.6434
10	2	4	4.8327	4.9627	11	5	2	6.4426	6.2920	14	0	2	2.0976	1.9276
10	2	5	26.0088	26.0849	11	5	3	2.3240	2.2114	14	0	3	4.4083	4.4037
10	2	6	27.2643	27.3991	11	5	4	3.6467	3.4310	14	0	4	9.5598	9.7656
10	2	7	7.7134	7.9588	11	5	5	4.7305	4.5811	14	0	5	5.4261	5.1559
10	2	8	17.2747	17.3354	11	5	6	9.7738	9.9260	14	0	6	6.3125	6.3064
10	2	9	2.0309	1.3285	11	5	7	16.5405	16.4852	14	2	0	12.6192	12.5848
10	2	10	18.1663	18.4501	11	5	8	4.9371	4.8138	14	2	1	21.7093	21.5453
10	2	11	6.5764	6.6648	11	5	9	17.5203	17.3123	14	2	2	20.9068	20.9935
10	2	12	5.2674	5.5463	12	0	0	5.1856	5.1875	14	2	3	7.0460	6.7979
10	2	13	12.6585	12.8446	12	0	1	15.8097	15.9226	14	2	4	3.8955	3.9643
10	2	14	15.9747	15.6319	12	0	2	2.1165	1.4089					
10	2	15	16.0530	15.6102	12	0	3	19.0233	18.9919					
10	4	0	19.7939	19.9547	12	0	4	24.4983	24.7624					
10	4	1	4.8815	4.7047	12	0	5	5.2133	5.1015					
10	4	2	13.9774	14.0158	12	0	6	11.1852	11.3747					
10	4	3	17.9602	18.1445	12	0	7	3.5877	3.2958					
10	4	4	26.5671	26.5815	12	0	8	13.6015	13.5982					
10	4	5	31.4224	31.2439	12	0	9	10.8321	10.9157					
10	4	6	2.4853	2.4746	12	0	10	4.3360	4.3089					
10	4	7	8.0399	7.7758	12	0	12	19.6934	19.5628					
10	4	8	4.3366	4.2996	12	2	0	1.8437	1.8185					
10	4	9	5.8350	5.6746	12	2	1	11.7199	11.8200					
10	4	10	1.9625	1.1011	12	2	2	21.4817	21.3858					
10	4	11	18.8183	18.7814	12	2	3	13.6452	13.5398					
10	4	12	15.6782	15.6862	12	2	4	16.5338	16.4251					
10	4	13	13.1167	13.0162	12	2	5	3.1309	2.9310					
10	6	1	4.5203	4.5570	12	2	6	15.8934	16.0854					
10	6	2	9.5348	9.5898	12	2	7	2.0263	1.2832					
10	6	3	4.4166	4.6934	12	2	8	7.2925	6.8939					
10	6	4	2.8850	2.4846	12	2	9	9.7939	9.8283					
10	6	5	19.3991	19.2550	12	2	10	7.7356	7.7696					
10	6	6	19.4004	19.3840	12	2	11	4.0931	3.9113					
10	6	7	3.5763	3.7963	12	4	0	5.4043	5.4945					
10	6	8	11.5092	11.5402	12	4	1	13.3338	13.6148					
11	1	0	5.8622	5.8990	12	4	3	16.0468	15.7398					
11	1	1	24.1354	24.3687	12	4	4	19.8849	19.8963					
11	1	2	8.6854	8.4942	12	4	5	3.9090	3.6240					
11	1	3	1.7182	0.9897	12	4	6	8.9692	8.8542					
11	1	4	8.2089	8.1971	12	4	7	2.9415	2.8855					
11	1	5	3.8103	3.6955	12	4	8	12.6026	12.6884					
11	1	6	11.8432	12.0330	12	4	9	9.4471	9.4082					
11	1	7	17.9100	17.9726	13	1	0	5.5584	5.5312					
11	1	8	3.6752	3.6620	13	1	1	5.3777	5.3803					
11	1	9	21.6367	21.7989	13	1	2	3.2860	2.9774					
11	1	10	3.6697	3.7035	13	1	3	12.3364	12.3670					
11	1	11	4.9663	5.0347	13	1	4	3.3071	2.8657					
11	1	12	11.5811	11.7648	13	1	5	14.2644	14.3101					
11	1	13	2.1106	1.9219	13	1	6	3.3774	3.1646					
11	3	0	2.5207	2.1205	13	1	7	2.5400	2.4800					
11	3	1	18.7658	18.8942	13	1	8	3.9400	4.1553					
11	3	2	7.8336	7.7710	13	1	9	2.7752	2.4118					
11	3	3	4.4588	4.3537	13	1	10	4.0373	3.6493					
11	3	4	10.7999	10.7188	13	3	1	6.6880	6.4689					
11	3	6	10.2102	10.1842	13	3	2	3.7198	3.4167					
11	3	7	12.6795	12.6320	13	3	3	13.4660	13.4829					

NU= 865 NV= 0

DISCREPANCY FACTORS BASED ON PARAMETERS BEFORE CYCLE 1

SUM(W*(O-C)**2) IS 0.5626E+03

SQRT(SUM(W*(O-C)**2/NU-NV) IS 0.8065

R FACTOR INCLUDING ZEROS

R FACTOR OMITTING ZEROS

WEIGHTED R FACTOR INCLUDING ZEROS

WEIGHTED R FACTOR OMITTING ZEROS

NUMERATOR	DENOMINATOR	R
1259.021	49272.887	0.026
1259.021	49272.887	0.026
23.720	668.583	0.035
23.720	668.583	0.035