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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, $V$ = 675.8Å, $Z$ = 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 $Ca^{6} - O$ = 2.421Å. 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 ($\lambda AgK\alpha$ = 0.56083Å), 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 $\sin\theta/\lambda$ = 0.84Å$^{-1}$. 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 $0kl$ 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 | 94.5195 |
| 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 | 64.3956 | 60.8620 |
| 0 | 2 | 4 | 21.6407 | 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 | 5.4569 | 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 | 23.2595 |
| 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 | 1.5780 | 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 | 15.5920 | 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 | 5.5687 | 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 | 33.8633 | 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 | 33.5967 | 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 | 7.8338 | 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 |

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|---|---|---|---|---|
| 2 | 4 | 12 | 31.7849 | 32.6768 |
| 2 | 4 | 13 | 8.5360 | 8.6651 |
| 2 | 4 | 14 | 2.3939 | 2.0740 |
| 2 | 4 | 15 | 8.1642 | 8.1507 |
| 2 | 4 | 16 | 5.1743 | 5.1693 |
| 2 | 4 | 17 | 7.2813 | 6.9827 |
| 2 | 4 | 18 | 16.0450 | 15.7016 |
| 2 | 5 | 0 | 33.4474 | 32.9579 |
| 2 | 6 | 2 | 18.8354 | 18.5986 |
| 2 | 6 | 3 | 24.3187 | 24.1116 |
| 2 | 6 | 4 | 4.5295 | 3.9510 |
| 2 | 6 | 5 | 5.3270 | 5.2316 |
| 2 | 6 | 6 | 26.7054 | 27.0410 |
| 2 | 6 | 7 | 7.8296 | 7.9345 |
| 2 | 6 | 8 | 28.5143 | 29.0707 |
| 2 | 6 | 9 | 8.7499 | 8.6995 |
| 2 | 6 | 10 | 10.0746 | 10.2529 |
| 2 | 6 | 11 | 5.5699 | 5.5877 |
| 2 | 6 | 13 | 8.9733 | 8.9975 |
| 2 | 6 | 14 | 19.9791 | 19.9896 |
| 2 | 6 | 15 | 4.7107 | 4.6448 |
| 2 | 6 | 16 | 12.8731 | 12.7007 |
| 2 | 6 | 17 | 7.8893 | 7.5574 |
| 2 | 8 | 0 | 2.9128 | 3.0615 |
| 2 | 8 | 1 | 8.0737 | 8.1397 |
| 2 | 8 | 2 | 12.1443 | 12.2350 |
| 2 | 8 | 3 | 9.2397 | 9.2549 |
| 2 | 8 | 4 | 28.6494 | 28.8639 |
| 2 | 8 | 5 | 7.7814 | 7.6622 |
| 2 | 8 | 6 | 4.1399 | 4.3199 |
| 2 | 8 | 7 | 15.7424 | 15.6288 |
| 2 | 8 | 9 | 9.3058 | 9.2313 |
| 2 | 8 | 10 | 11.2211 | 11.0936 |
| 2 | 8 | 11 | 3.5238 | 3.4944 |
| 2 | 8 | 12 | 18.6533 | 18.5322 |
| 3 | 1 | 0 | 76.9769 | 73.2220 |
| 3 | 1 | 1 | 14.2665 | 13.8756 |
| 3 | 1 | 2 | 43.9367 | 41.0333 |
| 3 | 1 | 3 | 9.7826 | 8.9729 |
| 3 | 1 | 4 | 14.9323 | 14.0969 |
| 3 | 1 | 5 | 11.2608 | 10.6368 |
| 3 | 1 | 6 | 12.5554 | 12.9149 |
| 3 | 1 | 7 | 3.5656 | 3.2470 |
| 3 | 1 | 8 | 46.9881 | 49.3035 |
| 3 | 1 | 9 | 14.4981 | 14.8946 |
| 3 | 1 | 10 | 33.3351 | 35.4968 |
| 3 | 1 | 11 | 7.0254 | 7.3707 |
| 3 | 1 | 12 | 4.6568 | 4.6878 |
| 3 | 1 | 13 | 6.3326 | 6.4089 |
| 3 | 1 | 14 | 9.5003 | 9.9193 |
| 3 | 1 | 15 | 2.8490 | 3.2120 |
| 3 | 1 | 16 | 18.0535 | 18.0253 |
| 3 | 1 | 18 | 20.6403 | 20.2423 |
| 3 | 1 | 20 | 8.4954 | 8.1913 |
| 3 | 1 | 21 | 5.2648 | 4.7298 |
| 3 | 3 | 0 | 68.7821 | 66.9670 |
| 3 | 3 | 1 | 2.2898 | 1.7680 |
| 3 | 3 | 2 | 30.3503 | 28.7600 |
| 3 | 3 | 3 | 1.9642 | 1.2148 |
| 3 | 3 | 4 | 3.6488 | 3.5817 |
| 3 | 3 | 5 | 4.4277 | 4.7958 |

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|---|---|---|---|---|
| 3 | 3 | 6 | 11.7304 | 11.7744 |
| 3 | 3 | 7 | 5.1566 | 4.8172 |
| 3 | 3 | 8 | 46.2373 | 48.2819 |
| 3 | 3 | 9 | 9.5948 | 9.9581 |
| 3 | 3 | 10 | 26.6044 | 27.9499 |
| 3 | 3 | 12 | 8.3622 | 8.5370 |
| 3 | 3 | 13 | 5.0738 | 5.1351 |
| 3 | 3 | 14 | 10.7714 | 11.2480 |
| 3 | 3 | 16 | 19.0087 | 18.8533 |
| 3 | 3 | 18 | 16.8118 | 16.3656 |
| 3 | 3 | 19 | 5.5952 | 5.3560 |
| 3 | 3 | 20 | 6.2545 | 5.9505 |
| 3 | 5 | 0 | 33.5238 | 33.5655 |
| 3 | 5 | 1 | 10.6848 | 10.9074 |
| 3 | 5 | 2 | 20.6578 | 20.2603 |
| 3 | 5 | 3 | 11.2441 | 11.2664 |
| 3 | 5 | 4 | 6.7117 | 6.8104 |
| 3 | 5 | 5 | 10.9412 | 11.3187 |
| 3 | 5 | 6 | 5.0561 | 5.0897 |
| 3 | 5 | 7 | 6.3701 | 6.6597 |
| 3 | 5 | 8 | 27.0994 | 27.8461 |
| 3 | 5 | 9 | 10.5049 | 10.7241 |
| 3 | 5 | 10 | 24.7968 | 25.5025 |
| 3 | 5 | 11 | 9.5043 | 9.6355 |
| 3 | 5 | 13 | 5.7721 | 5.7209 |
| 3 | 5 | 14 | 5.3500 | 5.6178 |
| 3 | 5 | 15 | 5.1243 | 5.2073 |
| 3 | 5 | 16 | 11.5217 | 11.2693 |
| 3 | 5 | 18 | 17.9319 | 17.1775 |
| 3 | 7 | 0 | 34.9406 | 35.2703 |
| 3 | 7 | 1 | 1.6085 | 1.5071 |
| 3 | 7 | 2 | 13.2247 | 13.2425 |
| 3 | 7 | 3 | 1.9693 | 1.8882 |
| 3 | 7 | 4 | 6.9169 | 6.6696 |
| 3 | 7 | 5 | 2.2380 | 2.2309 |
| 3 | 7 | 6 | 6.7054 | 6.7151 |
| 3 | 7 | 7 | 5.7713 | 5.6704 |
| 3 | 7 | 8 | 29.3949 | 29.6101 |
| 3 | 7 | 9 | 4.2057 | 4.1786 |
| 3 | 7 | 10 | 15.0800 | 15.2941 |
| 3 | 7 | 12 | 7.0110 | 7.0821 |
| 3 | 7 | 13 | 3.2571 | 3.1618 |
| 3 | 7 | 14 | 8.9694 | 9.1238 |
| 3 | 9 | 0 | 14.0962 | 14.4032 |
| 3 | 9 | 1 | 6.0649 | 5.9837 |
| 3 | 9 | 2 | 10.0872 | 10.1822 |
| 3 | 9 | 3 | 7.3956 | 7.4370 |
| 3 | 9 | 4 | 5.3607 | 5.4951 |
| 3 | 9 | 5 | 7.2383 | 7.0827 |
| 3 | 9 | 6 | 2.2462 | 2.2219 |
| 3 | 9 | 7 | 4.8666 | 4.7745 |
| 4 | 0 | 0 | 35.5361 | 33.6137 |
| 4 | 0 | 1 | 16.4872 | 15.8072 |
| 4 | 0 | 2 | 17.5669 | 17.5103 |
| 4 | 0 | 3 | 56.1802 | 55.3217 |
| 4 | 0 | 4 | 16.2770 | 14.5998 |
| 4 | 0 | 5 | 33.8307 | 33.8926 |
| 4 | 0 | 6 | 69.5118 | 72.0142 |
| 4 | 0 | 7 | 20.7708 | 21.1326 |
| 4 | 0 | 8 | 32.6222 | 34.3015 |
| 4 | 0 | 9 | 8.7471 | 9.7047 |

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|---|---|---|---|---|
| 4 | 0 | 10 | 25.3602 | 26.0793 |
| 4 | 0 | 11 | 18.1694 | 18.5170 |
| 4 | 0 | 12 | 11.1264 | 11.3676 |
| 4 | 0 | 13 | 26.1212 | 26.6763 |
| 4 | 0 | 14 | 37.3777 | 38.0127 |
| 4 | 0 | 15 | 9.5808 | 9.7149 |
| 4 | 0 | 16 | 4.0688 | 3.9144 |
| 4 | 0 | 17 | 5.3783 | 5.1392 |
| 4 | 0 | 18 | 3.7675 | 3.6777 |
| 4 | 0 | 19 | 10.3749 | 10.1212 |
| 4 | 0 | 21 | 11.1883 | 10.6401 |
| 4 | 2 | 0 | 19.3717 | 19.0956 |
| 4 | 2 | 1 | 17.8020 | 16.4581 |
| 4 | 2 | 2 | 39.5546 | 37.5719 |
| 4 | 2 | 3 | 42.3699 | 42.5527 |
| 4 | 2 | 4 | 96.3848 | 99.3229 |
| 4 | 2 | 5 | 28.2498 | 28.5063 |
| 4 | 2 | 6 | 3.1052 | 2.8666 |
| 4 | 2 | 7 | 21.9870 | 22.3366 |
| 4 | 2 | 8 | 18.9948 | 20.1806 |
| 4 | 2 | 9 | 8.6379 | 8.9019 |
| 4 | 2 | 10 | 2.3195 | 2.0623 |
| 4 | 2 | 11 | 13.4950 | 14.0556 |
| 4 | 2 | 12 | 44.1197 | 45.7041 |
| 4 | 2 | 13 | 25.4785 | 25.9173 |
| 4 | 2 | 14 | 7.5173 | 7.6058 |
| 4 | 2 | 15 | 10.9361 | 10.9460 |
| 4 | 2 | 16 | 7.8818 | 7.7271 |
| 4 | 2 | 17 | 4.3869 | 4.1859 |
| 4 | 2 | 18 | 11.4415 | 10.9577 |
| 4 | 2 | 19 | 8.7179 | 8.2804 |
| 4 | 2 | 20 | 22.8356 | 21.5591 |
| 4 | 4 | 1 | 8.4025 | 7.3436 |
| 4 | 4 | 2 | 16.1962 | 15.9305 |
| 4 | 4 | 3 | 33.0742 | 33.9473 |
| 4 | 4 | 4 | 5.1811 | 4.9046 |
| 4 | 4 | 5 | 23.5675 | 23.2425 |
| 4 | 4 | 6 | 47.9113 | 48.5764 |
| 4 | 4 | 7 | 13.4092 | 13.6550 |
| 4 | 4 | 8 | 29.1509 | 29.7340 |
| 4 | 4 | 9 | 6.2857 | 6.2289 |
| 4 | 4 | 10 | 19.5625 | 19.8597 |
| 4 | 4 | 11 | 14.0259 | 14.1782 |
| 4 | 4 | 12 | 7.2637 | 7.2824 |
| 4 | 4 | 13 | 21.1039 | 21.4078 |
| 4 | 4 | 14 | 29.1725 | 29.3692 |
| 4 | 4 | 15 | 7.3708 | 7.9413 |
| 4 | 4 | 16 | 4.1664 | 3.9970 |
| 4 | 4 | 17 | 4.4483 | 4.3312 |
| 4 | 4 | 18 | 3.3133 | 2.8993 |
| 4 | 4 | 19 | 9.1197 | 8.5729 |
| 4 | 6 | 0 | 11.0645 | 11.2851 |
| 4 | 6 | 1 | 6.5625 | 6.3118 |
| 4 | 6 | 2 | 21.0909 | 21.1464 |
| 4 | 6 | 3 | 21.4901 | 21.7157 |
| 4 | 6 | 4 | 48.5718 | 48.9942 |
| 4 | 6 | 5 | 16.3629 | 16.1487 |
| 4 | 6 | 6 | 2.0579 | 1.8764 |
| 4 | 6 | 7 | 11.9087 | 11.9477 |
| 4 | 6 | 8 | 8.8690 | 8.7959 |
| 4 | 6 | 9 | 5.1040 | 5.0793 |

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|---|---|---|---|---|
| 4 | 6 | 10 | 3.0636 | 2.9900 |
| 4 | 6 | 11 | 9.0099 | 9.0550 |
| 4 | 6 | 12 | 27.0244 | 27.0107 |
| 4 | 6 | 13 | 17.4226 | 17.4395 |
| 4 | 6 | 14 | 4.5125 | 4.3846 |
| 4 | 6 | 15 | 7.7596 | 7.5805 |
| 4 | 6 | 16 | 6.9028 | 6.6956 |
| 4 | 8 | 0 | 6.1621 | 6.1342 |
| 4 | 8 | 1 | 3.4939 | 3.4867 |
| 4 | 8 | 2 | 7.7659 | 7.7445 |
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| 5 | 5 | 10 | 5.6123 | 5.6702 |
| 5 | 5 | 11 | 11.5190 | 11.4442 |
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| 5 | 5 | 13 | 2.2548 | 2.5048 |
| 5 | 5 | 14 | 9.8133 | 9.8242 |
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| 5 | 7 | 4 | 21.1994 | 21.3119 |
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| 5 | 9 | 1 | 6.3928 | 6.4215 |
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| 7 | 5 | 6 | 5.8904 | 5.8362 |
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| 8 | 0 | 7 | 19.7772 | 20.1427 |
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| 8 | 0 | 9 | 24.5479 | 25.2950 |
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| 8 | 0 | 16 | 18.6655 | 18.3891 |
| 8 | 0 | 17 | 16.1834 | 15.8531 |
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| 8 | 2 | 17 | 13.5767 | 13.3546 |
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| 11 | 3 | 12 | 13.3425 | 13.1856 |
| 11 | 5 | 0 | 6.9109 | 7.0774 |
| 11 | 5 | 1 | 20.3656 | 20.4268 |
| 11 | 5 | 2 | 6.4426 | 6.2920 |
| 11 | 5 | 3 | 2.3240 | 2.2114 |
| 11 | 5 | 4 | 3.6467 | 3.4310 |
| 11 | 5 | 5 | 4.7305 | 4.5811 |
| 11 | 5 | 6 | 9.7738 | 9.9260 |
| 11 | 5 | 7 | 16.5405 | 16.4852 |
| 11 | 5 | 8 | 4.9371 | 4.8138 |
| 11 | 5 | 9 | 17.5203 | 17.3123 |
| 12 | 0 | 0 | 5.1856 | 5.1875 |
| 12 | 0 | 1 | 15.8097 | 15.9226 |
| 12 | 0 | 2 | 2.1165 | 1.4089 |
| 12 | 0 | 3 | 19.0233 | 18.9919 |
| 12 | 0 | 4 | 24.4983 | 24.7624 |
| 12 | 0 | 5 | 5.2133 | 5.1015 |
| 12 | 0 | 6 | 11.1852 | 11.3747 |
| 12 | 0 | 7 | 3.5877 | 3.2959 |
| 12 | 0 | 8 | 13.6015 | 13.5982 |
| 12 | 0 | 9 | 10.8321 | 10.9157 |
| 12 | 0 | 10 | 4.3360 | 4.3089 |
| 12 | 0 | 12 | 19.6934 | 19.5628 |
| 12 | 2 | 0 | 1.8437 | 1.8185 |
| 12 | 2 | 1 | 11.7199 | 11.8200 |
| 12 | 2 | 2 | 21.4817 | 21.3858 |
| 12 | 2 | 3 | 13.6452 | 13.5398 |
| 12 | 2 | 4 | 16.5338 | 16.4251 |
| 12 | 2 | 5 | 3.1309 | 2.9310 |
| 12 | 2 | 6 | 15.8934 | 16.0854 |
| 12 | 2 | 7 | 2.0263 | 1.2832 |
| 12 | 2 | 8 | 7.2925 | 6.8939 |
| 12 | 2 | 9 | 9.7939 | 9.8283 |
| 12 | 2 | 10 | 7.7356 | 7.7696 |
| 12 | 2 | 11 | 4.0931 | 3.9113 |
| 12 | 4 | 0 | 5.4043 | 5.4945 |
| 12 | 4 | 1 | 13.3338 | 13.6148 |
| 12 | 4 | 3 | 16.0468 | 15.7398 |
| 12 | 4 | 4 | 19.8849 | 19.8963 |
| 12 | 4 | 5 | 3.9090 | 3.6240 |
| 12 | 4 | 6 | 8.9692 | 8.8542 |
| 12 | 4 | 7 | 2.9415 | 2.3855 |
| 12 | 4 | 8 | 12.6026 | 12.6884 |
| 12 | 4 | 9 | 9.4471 | 9.4082 |
| 13 | 1 | 0 | 5.5584 | 5.5312 |
| 13 | 1 | 1 | 5.3777 | 5.3803 |
| 13 | 1 | 2 | 3.2860 | 2.9774 |
| 13 | 1 | 3 | 12.3364 | 12.3670 |
| 13 | 1 | 4 | 3.3071 | 2.8657 |
| 13 | 1 | 5 | 14.2644 | 14.3101 |
| 13 | 1 | 6 | 3.3774 | 3.1646 |
| 13 | 1 | 7 | 2.5400 | 2.4800 |
| 13 | 1 | 8 | 3.9400 | 4.1553 |
| 13 | 1 | 9 | 2.7752 | 2.4118 |
| 13 | 1 | 10 | 4.0373 | 3.6493 |
| 13 | 3 | 1 | 6.6880 | 6.4689 |
| 13 | 3 | 2 | 3.7198 | 3.4167 |
| 13 | 3 | 3 | 13.4660 | 13.4829 |

| | | | | |
|---|---|---|---|---|
| 13 | 3 | 4 | 6.3122 | 6.1914 |
| 13 | 3 | 5 | 14.3433 | 14.6629 |
| 13 | 3 | 6 | 2.4505 | 2.1339 |
| 13 | 3 | 7 | 4.4305 | 4.2232 |
| 14 | 0 | 0 | 11.6024 | 11.5250 |
| 14 | 0 | 1 | 12.7986 | 12.6434 |
| 14 | 0 | 2 | 2.0976 | 1.9276 |
| 14 | 0 | 3 | 4.4083 | 4.4937 |
| 14 | 0 | 4 | 9.5538 | 9.7656 |
| 14 | 0 | 5 | 5.4261 | 5.1559 |
| 14 | 0 | 6 | 6.3125 | 6.3064 |
| 14 | 2 | 0 | 12.6192 | 12.5843 |
| 14 | 2 | 1 | 21.7093 | 21.5453 |
| 14 | 2 | 2 | 20.9068 | 20.9935 |
| 14 | 2 | 3 | 7.0460 | 6.7979 |
| 14 | 2 | 4 | 3.3955 | 3.9647 |

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 |