

AM-90-435

Crystal growth and structure of $K_2Al_2Si_3O_{10} \cdot KCl$: A new anhydrous zeolite-type phase with the edingtonite framework

Subrata Ghose, Yang Hexiong, Jerry R. Weidner

For deposit: Table 4

American Mineralogist, 75, 7-8, 947-950.

#5788
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TABLE 4

Crystal Growth and Structure of $K_2Al_2Si_3O_{10}\cdot KCl$:

A New Anhydrous Zeolite-type Phase With the Edingtonite Framework

FOR DEPOSIT

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Key Words: $K_2Al_2Si_3O_{10}\cdot KCl$, zeolite-type phase, crystal growth, structure

Table 4 : $K_2Al_2Si_3O_{10}\cdot KCl$: Observed
and calculated structure
factors.

Table 4.

 $K_2Al_2Si_3O_{10} \cdot xCl$

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|---|---|----------|----------|----------|----------|
| 0 | 0 | 1 | 40. 833 | 41. 184 | -41. 184 | 0. 000 |
| 0 | 0 | 2 | 103. 377 | 100. 843 | 100. 843 | 0. 000 |
| 0 | 0 | 3 | 29. 349 | 16. 441 | -16. 441 | 0. 000 |
| 0 | 0 | 4 | 99. 727 | 97. 380 | -97. 380 | 0. 000 |
| 0 | 0 | 5 | 30. 426 | 29. 292 | 29. 292 | 0. 000 |
| 0 | 0 | 6 | 4. 696 | 4. 986 | 4. 986 | 0. 000 |
| 0 | 0 | 7 | 12. 484 | 14. 046 | 14. 046 | 0. 000 |
| 0 | 0 | 8 | 97. 841 | 48. 609 | 98. 609 | 0. 000 |
| 1 | 0 | 0 | 12. 580 | 11. 742 | 0. 000 | 11. 748 |
| 1 | 0 | 1 | 55. 618 | 55. 565 | 0. 000 | -55. 565 |
| 1 | 0 | 2 | 17. 211 | 15. 887 | 0. 000 | 13. 887 |
| 1 | 0 | 3 | 35. 675 | 34. 508 | 0. 000 | -34. 508 |
| 1 | 0 | 4 | 4. 750 | 4. 904 | 0. 000 | 4. 904 |
| 1 | 0 | 5 | 12. 785 | 13. 184 | 0. 000 | -13. 184 |
| 1 | 0 | 6 | 9. 051 | 8. 812 | 0. 000 | -8. 812 |
| 1 | 0 | 7 | 53. 675 | 60. 978 | 60. 978 | 0. 000 |
| 1 | 0 | 8 | 19. 129 | 18. 640 | 3. 588 | 18. 291 |
| 1 | 1 | 1 | 99. 110 | 96. 494 | -12. 121 | -95. 720 |
| 1 | 1 | 2 | 9. 079 | 10. 142 | 8. 764 | 4. 804 |
| 1 | 1 | 3 | 33. 082 | 32. 385 | -32. 382 | -2. 010 |
| 1 | 1 | 4 | 31. 245 | 30. 684 | 30. 495 | -15. 374 |
| 1 | 1 | 5 | 54. 316 | 54. 193 | 15. 876 | 51. 616 |
| 1 | 1 | 6 | 10. 827 | 12. 648 | 10. 398 | -7. 265 |
| 1 | 1 | 7 | 27. 027 | 27. 858 | 26. 496 | 8. 397 |
| 1 | 1 | 8 | 17. 721 | 19. 467 | -19. 467 | 0. 000 |
| 1 | 2 | 0 | 15. 588 | 14. 049 | 4. 830 | -13. 176 |
| 1 | 2 | 1 | 15. 270 | 14. 002 | 5. 295 | 12. 936 |
| 1 | 2 | 2 | 23. 084 | 21. 897 | -10. 589 | -19. 168 |
| 1 | 2 | 3 | 21. 285 | 21. 410 | 16. 756 | -13. 328 |
| 1 | 2 | 4 | 7. 039 | 8. 370 | -5. 719 | -6. 112 |
| 1 | 2 | 5 | 18. 289 | 19. 028 | 0. 348 | -19. 026 |
| 1 | 2 | 6 | 5. 935 | 7. 869 | -7. 246 | -3. 068 |
| 1 | 2 | 7 | 81. 784 | 86. 494 | -86. 494 | 0. 000 |
| 1 | 2 | 8 | 83. 284 | 84. 680 | 58. 804 | 60. 932 |
| 1 | 3 | 0 | 60. 581 | 56. 705 | -25. 527 | 50. 634 |
| 1 | 3 | 1 | 41. 278 | 41. 387 | 9. 498 | 40. 282 |
| 1 | 3 | 2 | 30. 824 | 29. 653 | 29. 593 | 1. 987 |
| 1 | 3 | 3 | 29. 256 | 28. 894 | -4. 542 | -38. 623 |
| 1 | 3 | 4 | 17. 727 | 16. 844 | 14. 878 | -7. 859 |
| 1 | 3 | 5 | 28. 395 | 29. 569 | 15. 460 | -25. 206 |
| 1 | 3 | 6 | 18. 448 | 18. 865 | 13. 654 | 13. 018 |
| 1 | 3 | 7 | 36. 010 | 37. 736 | 37. 736 | 0. 000 |
| 1 | 3 | 8 | 11. 269 | 9. 523 | -5. 674 | 7. 648 |
| 1 | 4 | 0 | 18. 743 | 18. 446 | 13. 456 | -12. 617 |
| 1 | 4 | 1 | 23. 140 | 23. 415 | -23. 093 | 3. 867 |
| 1 | 4 | 2 | 22. 017 | 21. 562 | 1. 287 | -21. 524 |
| 1 | 4 | 3 | 10. 674 | 10. 884 | -10. 559 | -2. 640 |
| 1 | 4 | 4 | 12. 539 | 14. 051 | 2. 057 | -13. 909 |
| 1 | 4 | 5 | 9. 942 | 10. 574 | 10. 549 | 0. 728 |
| 1 | 4 | 6 | 5. 544 | 5. 699 | -4. 277 | -3. 741 |
| 1 | 4 | 7 | 6. 997 | 8. 361 | 8. 201 | 1. 825 |
| 1 | 5 | 0 | 46. 111 | 48. 067 | -48. 067 | 0. 000 |
| 1 | 5 | 1 | 41. 496 | 44. 061 | 3. 124 | -43. 950 |

SYNLEUCITE 4

| H. | K. | L. | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|----|----|----|---------|---------|----------|----------|
| 1 | 1 | 6 | 18. 641 | 18. 739 | 6. 137 | -12. 651 |
| 1 | 1 | 7 | 48. 671 | 47. 659 | 13. 749 | -44. 564 |
| 1 | 1 | 8 | 36. 788 | 36. 692 | 35. 721 | -2. 935 |
| 1 | 1 | 9 | 18. 678 | 19. 119 | 6. 745 | -15. 817 |
| 1 | 1 | 10 | 20. 113 | 20. 050 | 7. 874 | -16. 645 |
| 1 | 1 | 11 | 16. 274 | 16. 007 | 7. 643 | -10. 985 |
| 1 | 1 | 12 | 6. 699 | 6. 129 | 8. 125 | 0. 000 |
| 1 | 1 | 13 | 19. 733 | 20. 542 | -10. 987 | -17. 438 |
| 1 | 1 | 14 | 42. 871 | 44. 362 | 7. 273 | -43. 761 |
| 1 | 1 | 15 | 24. 866 | 23. 769 | -2. 075 | 22. 985 |
| 1 | 1 | 16 | 21. 205 | 21. 279 | 2. 874 | -21. 088 |
| 1 | 1 | 17 | 4. 063 | 4. 895 | 4. 625 | -1. 509 |
| 1 | 1 | 18 | 5. 567 | 5. 149 | -0. 326 | -5. 140 |
| 1 | 1 | 19 | 8. 132 | 8. 948 | 8. 948 | 0. 000 |
| 1 | 1 | 20 | 22. 079 | 22. 604 | -5. 761 | 21. 567 |
| 1 | 1 | 21 | 33. 243 | 34. 001 | 23. 665 | -4. 764 |
| 1 | 1 | 22 | 18. 619 | 19. 525 | -16. 142 | 10. 984 |
| 1 | 1 | 23 | 23. 220 | 23. 250 | 22. 696 | -5. 037 |
| 1 | 1 | 24 | 7. 207 | 8. 744 | 5. 687 | -5. 634 |
| 1 | 1 | 25 | 19. 747 | 20. 314 | 20. 359 | -0. 459 |
| 1 | 1 | 26 | 39. 222 | 40. 816 | 40. 816 | 0. 000 |
| 1 | 1 | 27 | 26. 159 | 27. 491 | -23. 401 | -14. 345 |
| 1 | 1 | 28 | 14. 686 | 14. 875 | 10. 239 | -10. 790 |
| 1 | 1 | 29 | 25. 195 | 23. 867 | -23. 686 | -3. 174 |
| 1 | 1 | 30 | 14. 623 | 14. 913 | 12. 259 | 8. 493 |
| 1 | 1 | 31 | 6. 165 | 7. 570 | -2. 873 | -7. 032 |
| 1 | 1 | 32 | 5. 890 | 6. 223 | -5. 066 | 3. 628 |
| 1 | 1 | 33 | 11. 281 | 12. 627 | 11. 560 | -5. 082 |
| 1 | 1 | 34 | 20. 353 | 20. 844 | 20. 491 | -3. 926 |
| 1 | 1 | 35 | 17. 614 | 18. 132 | 14. 864 | -17. 467 |
| 1 | 1 | 36 | 10. 174 | 10. 760 | 10. 312 | -3. 073 |
| 1 | 1 | 37 | 16. 598 | 16. 715 | 9. 625 | 12. 685 |
| 1 | 1 | 38 | 19. 225 | 19. 635 | -19. 635 | 0. 000 |
| 1 | 1 | 39 | 8. 222 | 10. 391 | 1. 744 | -10. 244 |
| 1 | 1 | 40 | 15. 470 | 15. 250 | 3. 079 | 5. 439 |
| 1 | 1 | 41 | 22. 715 | 20. 817 | 18. 661 | -9. 227 |
| 1 | 1 | 42 | 16. 728 | 16. 414 | -5. 298 | 15. 535 |
| 1 | 1 | 43 | 17. 188 | 17. 949 | -17. 186 | -17. 910 |
| 1 | 1 | 44 | 10. 923 | 11. 648 | 0. 892 | 11. 613 |
| 1 | 1 | 45 | 19. 072 | 18. 799 | 17. 059 | 7. 878 |
| 1 | 1 | 46 | 6. 310 | 7. 133 | 1. 210 | 7. 030 |
| 1 | 1 | 47 | 4. 891 | 6. 370 | 6. 263 | 1. 165 |
| 1 | 1 | 48 | 6. 450 | 6. 162 | 1. 139 | -6. 055 |
| 1 | 1 | 49 | 18. 079 | 17. 677 | -17. 677 | 0. 000 |
| 1 | 1 | 50 | 17. 307 | 17. 813 | 13. 572 | 11. 538 |
| 1 | 1 | 51 | 6. 611 | 8. 314 | -1. 354 | -9. 202 |
| 1 | 1 | 52 | 14. 283 | 14. 393 | -8. 553 | 11. 576 |
| 1 | 1 | 53 | 14. 708 | 14. 708 | 12. 634 | -7. 531 |
| 1 | 1 | 54 | 10. 776 | 11. 180 | -10. 140 | -4. 708 |
| 1 | 1 | 55 | 6. 270 | 9. 397 | 9. 137 | -2. 194 |
| 1 | 1 | 56 | 10. 537 | 11. 212 | 11. 109 | -1. 517 |
| 1 | 1 | 57 | 8. 971 | 11. 926 | 11. 926 | 0. 000 |

SYNLEUCITE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|----|----|-----|---------|---------|---------|---------|
| -1 | 14 | 4 | 11.304 | 11.627 | -7.313 | 9.029 |
| -1 | 14 | 9 | 9.567 | 11.045 | 7.140 | 9.495 |
| -1 | 0 | 11 | 11.729 | 10.165 | 10.165 | 0.000 |
| 0 | 0 | 5 | 5.328 | 6.899 | 6.399 | 0.000 |
| 0 | 0 | 6 | 56.308 | 54.503 | 54.503 | 0.000 |
| 0 | 0 | 13 | 13.846 | 15.750 | 15.750 | 0.000 |
| 0 | 0 | 68 | 68.080 | 67.937 | 67.937 | 0.000 |
| 0 | 0 | 21 | 21.342 | 20.509 | 20.509 | 0.000 |
| 0 | 0 | 13 | 13.437 | 13.570 | 13.570 | 0.000 |
| 0 | 0 | 14 | 14.093 | 17.773 | -17.773 | 0.000 |
| 0 | 0 | 17 | 17.642 | 19.447 | 19.447 | 0.000 |
| 0 | 0 | 15 | 15.293 | 14.040 | 14.040 | 13.176 |
| 0 | 0 | 14 | 14.215 | 14.002 | -5.285 | -12.966 |
| 0 | 0 | 22 | 22.770 | 21.699 | 19.049 | 19.168 |
| 0 | 0 | 21 | 21.915 | 21.410 | -16.706 | 13.326 |
| 0 | 0 | 9 | 9.397 | 8.370 | 5.713 | 6.112 |
| 0 | 0 | 17 | 17.977 | 19.028 | -0.363 | 19.025 |
| 0 | 0 | 5 | 5.3 | 2.881 | -2.864 | -0.316 |
| 0 | 0 | 105 | 105.939 | 111.967 | 111.967 | 0.000 |
| 0 | 0 | 106 | 106.453 | 104.681 | 70.073 | 74.957 |
| 0 | 0 | 34 | 34.760 | 35.715 | 32.719 | -14.321 |
| 0 | 0 | 46 | 46.939 | 46.495 | 14.010 | 46.322 |
| 0 | 0 | 20 | 20.502 | 19.369 | -15.833 | -4.525 |
| 0 | 0 | 5 | 50.968 | 49.601 | -4.411 | -49.435 |
| 0 | 0 | 31 | 31.873 | 29.870 | 8.492 | 28.638 |
| 0 | 0 | 32 | 32.425 | 33.309 | 14.849 | -29.816 |
| 0 | 0 | 21 | 21.858 | 23.798 | 20.981 | 11.416 |
| 0 | 0 | 17 | 17.693 | 18.931 | 10.057 | 16.039 |
| 0 | 0 | 10 | 10.069 | 11.552 | -11.552 | 0.000 |
| 0 | 0 | 12 | 12.467 | 10.980 | 3.823 | -10.293 |
| 0 | 0 | 57 | 57.970 | 56.843 | 7.879 | 56.294 |
| 0 | 0 | 26 | 26.993 | 24.990 | -20.865 | -13.752 |
| 0 | 0 | 32 | 32.356 | 31.558 | 20.114 | 24.318 |
| 0 | 0 | 11 | 11.604 | 11.107 | -11.023 | -1.362 |
| 0 | 0 | 8 | 8.018 | 8.118 | 7.665 | 2.674 |
| 0 | 0 | 10 | 10.742 | 12.383 | -10.527 | 6.521 |
| 0 | 0 | 19 | 19.656 | 20.205 | -18.758 | 7.512 |
| 0 | 0 | 45 | 45.015 | 43.057 | 40.102 | 15.674 |
| 0 | 0 | 40 | 40.981 | 40.310 | 40.241 | -2.361 |
| 0 | 0 | 46 | 46.973 | 45.639 | 45.450 | -4.145 |
| 0 | 0 | 29 | 29.031 | 29.414 | 29.145 | -3.972 |
| 0 | 0 | 6 | 9.056 | 9.810 | 6.550 | -7.303 |
| 0 | 0 | 7 | 3.181 | 6.958 | -5.217 | 4.604 |
| 0 | 0 | 8 | 6.384 | 8.219 | -7.854 | 2.423 |
| 0 | 0 | 10 | 10.509 | 9.290 | 9.290 | 0.000 |
| 0 | 0 | 8 | 8.625 | 8.871 | 8.294 | 3.171 |
| 0 | 0 | 12 | 6.032 | 4.754 | 4.252 | 2.127 |
| 0 | 0 | 23 | 23.736 | 24.196 | -23.980 | 3.232 |
| 0 | 0 | 13 | 13.006 | 11.420 | 6.746 | 9.215 |
| 0 | 0 | 11 | 11.712 | 12.548 | -11.081 | 5.987 |
| 0 | 0 | 6 | 9.102 | 8.860 | 3.603 | 9.139 |
| 0 | 0 | 7 | 12.374 | 12.172 | 10.779 | 5.553 |

SYNLEUCYTE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|----|---|---|---------|---------|----------|----------|
| 5 | 0 | 8 | 5. 533 | 5. 240 | -9. 400 | 2. 332 |
| 6 | 0 | 9 | 65. 588 | 67. 614 | 67. 614 | 0. 000 |
| 6 | 1 | 0 | 37. 400 | 38. 802 | 10. 952 | -37. 824 |
| 6 | 1 | 1 | 60. 864 | 60. 486 | 38. 980 | 46. 382 |
| 6 | 2 | 0 | 36. 265 | 36. 390 | -0. 615 | -36. 385 |
| 6 | 2 | 1 | 11. 899 | 11. 442 | 2. 926 | 11. 061 |
| 6 | 3 | 0 | 13. 534 | 13. 497 | 1. 465 | 13. 417 |
| 6 | 3 | 1 | 21. 228 | 20. 759 | 3. 850 | -20. 587 |
| 6 | 4 | 0 | 16. 513 | 15. 847 | 11. 467 | 10. 938 |
| 6 | 4 | 1 | 8. 506 | 9. 410 | 9. 209 | -1. 787 |
| 7 | 0 | 7 | 35. 499 | 39. 548 | 29. 549 | 0. 000 |
| 7 | 0 | 8 | 23. 604 | 24. 262 | -24. 286 | -1. 789 |
| 7 | 1 | 0 | 18. 465 | 18. 311 | 0. 904 | 18. 269 |
| 7 | 1 | 1 | 17. 580 | 16. 002 | 15. 395 | -4. 364 |
| 7 | 2 | 0 | 34. 075 | 33. 740 | -29. 450 | 16. 465 |
| 7 | 2 | 1 | 20. 542 | 19. 981 | 18. 337 | -7. 938 |
| 7 | 3 | 0 | 8. 080 | 9. 274 | -2. 049 | 9. 045 |
| 7 | 3 | 1 | 8. 671 | 9. 710 | -7. 408 | -6. 277 |
| 7 | 4 | 0 | 14. 910 | 15. 275 | 14. 323 | 5. 307 |
| 7 | 4 | 1 | 13. 519 | 15. 161 | 15. 161 | 0. 000 |
| 8 | 0 | 6 | 32. 861 | 33. 472 | 19. 577 | -27. 089 |
| 8 | 0 | 7 | 12. 370 | 11. 773 | 11. 762 | 0. 523 |
| 8 | 1 | 0 | 22. 408 | 21. 381 | 21. 122 | 3. 321 |
| 8 | 1 | 1 | 11. 304 | 11. 712 | 11. 691 | -1. 195 |
| 8 | 2 | 0 | 19. 160 | 19. 052 | 8. 227 | 17. 184 |
| 8 | 2 | 1 | 5. 555 | 6. 594 | 4. 064 | -5. 193 |
| 8 | 3 | 0 | 3. 796 | 3. 058 | 3. 058 | 0. 000 |
| 8 | 3 | 1 | 12. 586 | 14. 722 | -14. 188 | -3. 927 |
| 8 | 4 | 0 | 5. 748 | 6. 350 | 4. 803 | -4. 163 |
| 8 | 4 | 1 | 7. 127 | 8. 360 | 5. 863 | -5. 559 |
| 8 | 5 | 0 | 13. 227 | 13. 217 | 1. 118 | 13. 169 |
| 8 | 5 | 1 | 18. 293 | 17. 121 | -3. 080 | 16. 842 |
| 9 | 0 | 6 | 5. 877 | 6. 116 | -3. 984 | -4. 641 |
| 9 | 0 | 7 | 24. 343 | 24. 514 | 24. 514 | 0. 000 |
| 9 | 1 | 0 | 12. 926 | 12. 810 | 9. 929 | 8. 094 |
| 9 | 1 | 1 | 23. 192 | 23. 315 | 21. 253 | -9. 588 |
| 9 | 2 | 0 | 12. 308 | 12. 900 | -9. 834 | 8. 346 |
| 9 | 2 | 1 | 13. 500 | 13. 407 | 13. 386 | -0. 755 |
| 9 | 3 | 0 | 5. 754 | 6. 395 | -3. 972 | -5. 012 |
| 9 | 3 | 1 | 6. 162 | 6. 652 | 4. 654 | 4. 752 |
| 9 | 4 | 0 | 11. 718 | 13. 665 | 12. 617 | -5. 247 |
| 9 | 4 | 1 | 33. 423 | 32. 154 | -32. 154 | 0. 000 |
| 10 | 0 | 0 | 14. 952 | 15. 446 | 15. 401 | 1. 188 |
| 10 | 0 | 1 | 7. 252 | 7. 916 | -1. 581 | 7. 756 |
| 10 | 1 | 0 | 763 | 9. 151 | -9. 119 | -0. 769 |
| 10 | 1 | 1 | 108. | 23. 614 | 23. 048 | 5. 137 |
| 10 | 2 | 0 | 13. 170 | 14. 123 | -13. 397 | -4. 489 |
| 10 | 2 | 1 | 19. 265 | 18. 587 | 18. 587 | 0. 000 |
| 10 | 3 | 0 | 5. 629 | 7. 226 | -6. 679 | -2. 759 |
| 10 | 3 | 1 | 13. 420 | 13. 956 | 12. 878 | 5. 379 |
| 10 | 4 | 0 | 8. 404 | 8. 998 | 8. 298 | -3. 480 |
| 10 | 4 | 1 | 6. 667 | 9. 496 | 9. 457 | 0. 739 |
| 10 | 5 | 0 | 4. 693 | 5. 481 | 2. 930 | -4. 632 |

SYNLEUCITE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|----|---|----|--------|---------|---------|---------|
| 13 | 0 | 4 | 5.923 | 5.508 | -1.462 | 9.295 |
| 13 | 0 | 7 | 7.354 | 8.113 | -0.418 | -8.102 |
| 13 | 0 | 4 | 4.630 | 5.650 | 1.568 | 5.453 |
| 13 | 0 | 9 | 9.391 | 10.728 | 10.728 | 0.000 |
| 13 | 0 | 4 | 4.469 | 6.019 | 0.000 | 6.019 |
| 13 | 0 | 42 | 42.503 | 40.521 | 0.000 | -40.521 |
| 13 | 0 | 23 | 23.180 | 22.507 | 0.000 | -22.507 |
| 13 | 0 | 40 | 40.351 | 39.409 | 0.000 | -39.409 |
| 13 | 0 | 15 | 15.662 | 15.655 | 0.000 | 15.645 |
| 13 | 0 | 21 | 21.361 | 23.531 | 0.000 | -23.531 |
| 13 | 0 | 4 | 4.619 | 3.840 | 0.000 | 3.840 |
| 13 | 0 | 8 | 8.832 | 11.101 | 0.000 | -11.101 |
| 13 | 0 | 4 | 4.551 | 3.842 | 0.000 | 3.842 |
| 13 | 1 | 1 | 85.168 | 86.494 | -86.494 | 0.000 |
| 13 | 1 | 93 | 93.721 | 94.680 | -58.804 | 60.922 |
| 13 | 1 | 59 | 59.877 | 54.705 | -25.827 | 50.684 |
| 13 | 1 | 42 | 42.292 | 41.387 | 9.498 | 40.282 |
| 13 | 1 | 30 | 30.404 | 29.653 | 29.653 | 1.587 |
| 13 | 1 | 39 | 39.545 | 38.889 | -4.542 | -38.623 |
| 13 | 1 | 17 | 17.511 | 16.844 | 14.848 | -7.859 |
| 13 | 1 | 28 | 28.463 | 29.569 | 15.460 | -25.206 |
| 13 | 1 | 4 | 4.591 | 5.460 | 1.085 | 5.290 |
| 13 | 1 | 19 | 19.260 | 18.866 | 13.654 | 13.019 |
| 13 | 1 | 9 | 9.805 | 11.552 | 11.552 | 0.000 |
| 13 | 1 | 12 | 12.041 | 10.980 | -3.823 | 10.293 |
| 13 | 1 | 57 | 57.545 | 56.843 | -7.879 | -56.294 |
| 13 | 1 | 24 | 24.399 | 24.970 | 20.865 | 13.752 |
| 13 | 1 | 31 | 31.244 | 31.558 | -20.114 | -24.318 |
| 13 | 1 | 12 | 12.618 | 11.106 | 11.023 | 1.362 |
| 13 | 1 | 7 | 7.297 | 8.118 | -7.665 | -2.674 |
| 13 | 1 | 9 | 9.771 | 12.383 | 10.527 | -6.521 |
| 13 | 1 | 6 | 6.104 | 7.120 | -7.006 | 1.268 |
| 13 | 1 | 30 | 30.461 | 29.788 | -29.788 | 0.000 |
| 13 | 1 | 27 | 27.737 | 25.064 | 18.632 | 14.764 |
| 13 | 1 | 2 | 42.848 | 40.691 | -26.623 | -30.774 |
| 13 | 1 | 3 | 50.128 | 48.797 | 48.181 | 7.855 |
| 13 | 1 | 4 | 22.204 | 21.503 | -16.337 | 13.980 |
| 13 | 1 | 5 | 32.725 | 31.818 | 31.700 | -2.737 |
| 13 | 1 | 6 | 19.038 | 18.784 | 11.043 | 15.175 |
| 13 | 1 | 7 | 7.978 | 9.153 | -5.710 | 7.153 |
| 13 | 1 | 8 | 26.125 | 25.259 | 24.672 | 5.410 |
| 13 | 1 | 9 | 5.862 | 8.851 | -7.839 | 4.109 |
| 13 | 1 | 10 | 18.885 | 19.030 | -19.030 | 0.000 |
| 13 | 1 | 11 | 14.373 | 15.318 | 14.659 | -4.444 |
| 13 | 1 | 12 | 8.966 | 7.337 | 3.993 | 6.135 |
| 13 | 1 | 13 | 19.100 | 17.988 | -17.812 | -2.511 |
| 13 | 1 | 14 | 31.079 | 30.796 | 21.623 | -21.928 |
| 13 | 1 | 15 | 15.514 | 14.556 | -11.225 | 9.266 |
| 13 | 1 | 16 | 27.907 | 27.926 | 2.174 | -27.841 |
| 13 | 1 | 17 | 10.452 | 11.409 | 7.161 | 8.881 |
| 13 | 1 | 18 | 12.949 | 13.133 | -11.426 | -6.475 |
| 13 | 5 | 0 | 45.084 | 42.894 | 42.894 | 0.000 |
| 13 | 5 | 2 | 48.989 | 47.275 | -11.771 | 47.242 |

SYNLEUCITE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|----|---|---------|---------|----------|----------|
| 5 | 4 | 3 | 23. 623 | 23. 127 | 23. 950 | 2. 854 |
| 5 | 4 | 4 | 28. 922 | 28. 330 | -26. 319 | -0. 783 |
| 5 | 4 | 5 | 23. 963 | 23. 011 | 22. 095 | 6. 427 |
| 5 | 4 | 6 | 23. 564 | 23. 749 | 3. 494 | -31. 574 |
| 5 | 4 | 7 | 6. 464 | 6. 252 | 3. 743 | -4. 993 |
| 5 | 4 | 8 | 23. 540 | 23. 240 | 24. 711 | -4. 065 |
| 5 | 4 | 9 | 10. 814 | 10. 866 | 10. 864 | 0. 000 |
| 5 | 5 | 0 | 20. 621 | 22. 126 | 19. 547 | -10. 367 |
| 5 | 5 | 1 | 15. 247 | 15. 702 | -6. 591 | 13. 143 |
| 5 | 5 | 2 | 11. 122 | 10. 412 | -4. 283 | -9. 491 |
| 5 | 5 | 3 | 19. 503 | 20. 341 | -13. 433 | -15. 274 |
| 5 | 5 | 4 | 11. 593 | 12. 054 | -3. 018 | 11. 650 |
| 5 | 5 | 5 | 25. 285 | 25. 157 | 4. 094 | -25. 835 |
| 5 | 5 | 6 | 12. 660 | 12. 626 | 3. 748 | 12. 265 |
| 5 | 5 | 7 | 36. 721 | 37. 082 | -27. 082 | 0. 000 |
| 5 | 5 | 8 | 38. 959 | 40. 052 | 33. 982 | -21. 199 |
| 5 | 5 | 9 | 21. 903 | 22. 927 | -4. 829 | -22. 413 |
| 5 | 6 | 0 | 15. 089 | 15. 709 | -1. 751 | -15. 692 |
| 5 | 6 | 1 | 29. 048 | 28. 100 | 27. 698 | 4. 740 |
| 5 | 6 | 2 | 12. 350 | 12. 553 | -1. 290 | 12. 432 |
| 5 | 6 | 3 | 19. 804 | 19. 603 | 21. 617 | 15. 790 |
| 5 | 6 | 4 | 14. 239 | 14. 656 | 13. 633 | 5. 380 |
| 5 | 6 | 5 | 11. 417 | 11. 465 | 31. 465 | 0. 000 |
| 5 | 6 | 6 | 19. 561 | 19. 468 | -19. 063 | 13. 465 |
| 5 | 6 | 7 | 19. 951 | 20. 812 | 1. 553 | -20. 754 |
| 5 | 6 | 8 | 16. 984 | 17. 684 | 14. 159 | 10. 597 |
| 5 | 6 | 9 | 11. 281 | 10. 690 | -8. 971 | -5. 815 |
| 5 | 7 | 0 | 18. 305 | 17. 088 | 12. 097 | -12. 059 |
| 5 | 7 | 1 | 8. 262 | 9. 193 | -2. 197 | 8. 928 |
| 5 | 7 | 2 | 12. 489 | 12. 646 | -7. 837 | -9. 926 |
| 5 | 7 | 3 | 24. 741 | 25. 248 | 20. 215 | 15. 126 |
| 5 | 7 | 4 | 13. 301 | 14. 001 | 1. 449 | -13. 926 |
| 5 | 7 | 5 | 18. 504 | 18. 024 | 0. 593 | 18. 014 |
| 5 | 7 | 6 | 6. 679 | 7. 575 | 7. 438 | -1. 434 |
| 5 | 7 | 7 | 5. 323 | 4. 438 | -0. 342 | -4. 425 |
| 5 | 7 | 8 | 8. 733 | 8. 725 | 7. 504 | 4. 451 |
| 5 | 7 | 9 | 12. 450 | 12. 310 | 9. 921 | -7. 288 |
| 5 | 8 | 0 | 7. 360 | 10. 762 | 0. 699 | 10. 739 |
| 5 | 8 | 1 | 18. 283 | 17. 377 | 3. 234 | -17. 073 |
| 5 | 8 | 2 | 9. 272 | 11. 556 | -0. 738 | 11. 532 |
| 5 | 8 | 3 | 8. 888 | 10. 307 | 8. 083 | -6. 395 |
| 5 | 8 | 4 | 5. 317 | 6. 824 | -4. 067 | -5. 480 |
| 5 | 8 | 5 | 5. 924 | 5. 479 | -1. 793 | 5. 178 |
| 5 | 8 | 6 | 5. 578 | 6. 839 | 6. 939 | 0. 000 |
| 5 | 9 | 0 | 6. 736 | 8. 581 | -2. 800 | -8. 112 |
| 5 | 9 | 1 | 10. 135 | 10. 556 | 5. 584 | 8. 958 |
| 5 | 9 | 2 | 15. 184 | 15. 404 | 12. 219 | -9. 379 |
| 5 | 9 | 3 | 10. 015 | 11. 309 | 10. 829 | 3. 264 |
| 5 | 10 | 0 | 15. 400 | 15. 418 | -15. 418 | 0. 000 |
| 5 | 10 | 1 | 7. 190 | 9. 561 | 4. 946 | -8. 182 |
| 5 | 10 | 2 | 5. 328 | 8. 036 | -0. 906 | -7. 985 |
| 5 | 10 | 3 | 9. 641 | 11. 479 | 11. 479 | 0. 042 |
| 5 | 10 | 4 | 5. 396 | 6. 391 | -3. 871 | 5. 085 |

SYNLEUCITE Z

| H. | K. | L. | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|----|----|----|---------|---------|---------|---------|
| 3 | 13 | 0 | 4.262 | 2.930 | 2.930 | 0.000 |
| 3 | 13 | 1 | 4.647 | 6.152 | 6.152 | 2.157 |
| 3 | 13 | 3 | 5.987 | 7.749 | 7.749 | 1.258 |
| 3 | 14 | 0 | 13.131 | 12.740 | 12.740 | 0.000 |
| 3 | 14 | 1 | 9.850 | 8.904 | -4.501 | -7.802 |
| 3 | 14 | 2 | 9.079 | 9.887 | 2.203 | 9.629 |
| 4 | 0 | 0 | 25.450 | 26.389 | 26.389 | 0.000 |
| 4 | 0 | 1 | 51.439 | 52.390 | 52.390 | 0.000 |
| 4 | 0 | 2 | 57.550 | 55.601 | 55.601 | 0.000 |
| 4 | 0 | 3 | 25.785 | 26.006 | -26.006 | 0.000 |
| 4 | 0 | 4 | 55.627 | 54.778 | 54.778 | 0.000 |
| 4 | 0 | 5 | 33.298 | 31.241 | -31.241 | 0.000 |
| 4 | 0 | 6 | 4.891 | 4.610 | 4.610 | 0.000 |
| 4 | 0 | 7 | 26.012 | 26.454 | 26.454 | 0.000 |
| 4 | 0 | 8 | 12.177 | 13.174 | -13.174 | 0.000 |
| 4 | 0 | 9 | 30.994 | 29.876 | 29.876 | 0.000 |
| 4 | 1 | 0 | 38.484 | 37.736 | -37.736 | 0.000 |
| 4 | 1 | 1 | 12.058 | 9.523 | 9.523 | 0.648 |
| 4 | 1 | 2 | 18.641 | 19.446 | -19.446 | 12.617 |
| 4 | 1 | 3 | 22.851 | 23.415 | 23.415 | -3.867 |
| 4 | 1 | 4 | 23.129 | 21.562 | -1.287 | 21.524 |
| 4 | 1 | 5 | 10.148 | 10.884 | 10.884 | 2.640 |
| 4 | 1 | 6 | 12.189 | 14.061 | -2.061 | 13.909 |
| 4 | 1 | 7 | 10.781 | 10.574 | -10.574 | -0.728 |
| 4 | 1 | 8 | 5.191 | 5.699 | 4.295 | 3.741 |
| 4 | 1 | 9 | 6.679 | 8.361 | -8.201 | -1.628 |
| 4 | 2 | 1 | 19.174 | 20.206 | -18.799 | -7.512 |
| 4 | 2 | 2 | 44.396 | 43.057 | 40.103 | 15.574 |
| 4 | 2 | 3 | 41.912 | 40.310 | 40.241 | -2.361 |
| 4 | 2 | 4 | 47.193 | 45.639 | 45.450 | -4.146 |
| 4 | 2 | 5 | 29.354 | 29.414 | 29.145 | -3.972 |
| 4 | 2 | 6 | 10.038 | 9.810 | 6.550 | -7.303 |
| 4 | 2 | 7 | 4.795 | 6.958 | -5.217 | 4.604 |
| 4 | 2 | 8 | 6.730 | 8.219 | -7.854 | 2.423 |
| 4 | 3 | 0 | 17.165 | 19.030 | 19.030 | 0.000 |
| 4 | 3 | 1 | 13.779 | 15.318 | -14.659 | 4.444 |
| 4 | 3 | 2 | 8.744 | 7.337 | -3.993 | -6.125 |
| 4 | 3 | 3 | 19.730 | 17.988 | 17.812 | 2.511 |
| 4 | 3 | 4 | 30.670 | 30.794 | -21.823 | 21.927 |
| 4 | 3 | 5 | 14.947 | 14.556 | 11.235 | -7.266 |
| 4 | 3 | 6 | 28.401 | 27.926 | -2.174 | 27.841 |
| 4 | 3 | 7 | 10.146 | 11.409 | -7.161 | -8.881 |
| 4 | 3 | 8 | 11.338 | 13.133 | 11.426 | 6.475 |
| 4 | 3 | 9 | 4.687 | 4.701 | -5.699 | 0.161 |
| 4 | 4 | 0 | 128.481 | 131.967 | 131.967 | 0.000 |
| 4 | 4 | 1 | 4.545 | 5.495 | 2.427 | 4.919 |
| 4 | 4 | 2 | 42.899 | 42.339 | 36.550 | 21.371 |
| 4 | 4 | 3 | 16.592 | 16.669 | 13.511 | 9.784 |
| 4 | 4 | 4 | 46.945 | 44.829 | -41.769 | -16.279 |
| 4 | 4 | 5 | 23.950 | 22.255 | 18.743 | 11.998 |
| 4 | 4 | 6 | 27.044 | 28.554 | 4.940 | -28.141 |
| 4 | 4 | 7 | 9.750 | 11.288 | 4.843 | 10.175 |
| 4 | 4 | 8 | 32.464 | 31.729 | 31.301 | -5.198 |

SYNLSUCITE #4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|----|----|--------|---------|---------|---------|
| 4 | 0 | 0 | 24.756 | 23.802 | -23.802 | 0.000 |
| 4 | 1 | 0 | 21.165 | 22.546 | 19.986 | -10.435 |
| 4 | 2 | 0 | 43.251 | 41.800 | -10.249 | 40.519 |
| 4 | 3 | 0 | 13.295 | 13.511 | -6.846 | -11.648 |
| 4 | 4 | 0 | 14.504 | 14.086 | 7.254 | 12.068 |
| 4 | 5 | 0 | 8.943 | 9.115 | -6.722 | 5.731 |
| 4 | 6 | 0 | 8.835 | 10.061 | 3.547 | -9.488 |
| 4 | 7 | 0 | 8.954 | 8.870 | 3.768 | 7.933 |
| 4 | 8 | 0 | 18.168 | 16.798 | 16.798 | 0.000 |
| 4 | 9 | 0 | 9.431 | 9.283 | 6.740 | -2.499 |
| 4 | 10 | 0 | 48.257 | 47.495 | 26.113 | -39.672 |
| 4 | 11 | 0 | 6.214 | 6.306 | 0.845 | 5.249 |
| 4 | 12 | 0 | 35.182 | 33.122 | 32.955 | -3.326 |
| 4 | 13 | 0 | 6.946 | 7.863 | 7.625 | 1.878 |
| 4 | 14 | 0 | 20.553 | 20.243 | 11.356 | 15.831 |
| 4 | 15 | 0 | 9.749 | 10.866 | 10.490 | -2.838 |
| 4 | 16 | 0 | 7.700 | 8.822 | -8.688 | -1.530 |
| 4 | 17 | 0 | 26.897 | 26.988 | -26.988 | 0.000 |
| 4 | 18 | 0 | 29.736 | 29.464 | 27.630 | -6.640 |
| 4 | 19 | 0 | 27.502 | 27.045 | -14.865 | 22.594 |
| 4 | 20 | 0 | 13.329 | 12.543 | -5.276 | -11.379 |
| 4 | 21 | 0 | 11.440 | 11.576 | 3.392 | 11.068 |
| 4 | 22 | 0 | 6.265 | 8.058 | -8.045 | -0.454 |
| 4 | 23 | 0 | 13.063 | 13.627 | 13.627 | 0.000 |
| 4 | 24 | 0 | 30.500 | 32.069 | 31.289 | 7.031 |
| 4 | 25 | 0 | 19.912 | 19.796 | 17.626 | -9.011 |
| 4 | 26 | 0 | 16.411 | 16.482 | -11.814 | 11.492 |
| 4 | 27 | 0 | 19.509 | 19.369 | 17.598 | -5.302 |
| 4 | 28 | 0 | 9.289 | 9.764 | -9.704 | 1.076 |
| 4 | 29 | 0 | 5.953 | 6.657 | 6.276 | -2.221 |
| 4 | 30 | 0 | 15.349 | 16.229 | 15.815 | -3.643 |
| 4 | 31 | 0 | 6.577 | 7.818 | 7.818 | 0.000 |
| 4 | 32 | 1 | 22.238 | 22.637 | -9.063 | 20.743 |
| 4 | 33 | 1 | 9.879 | 11.255 | -0.173 | -11.254 |
| 4 | 34 | 2 | 17.948 | 19.291 | 6.852 | 17.153 |
| 4 | 35 | 2 | 7.184 | 8.506 | -7.377 | 4.235 |
| 4 | 36 | 3 | 19.185 | 18.395 | 5.131 | -17.665 |
| 4 | 37 | 3 | 18.817 | 17.102 | -1.214 | 17.058 |
| 4 | 38 | 4 | 13.091 | 14.037 | -3.318 | -13.640 |
| 4 | 39 | 4 | 19.702 | 19.480 | 19.480 | 0.000 |
| 4 | 40 | 5 | 12.699 | 13.617 | -12.073 | -6.298 |
| 4 | 41 | 5 | 16.798 | 16.370 | 16.214 | -2.257 |
| 4 | 42 | 6 | 17.591 | 17.232 | 16.375 | -5.367 |
| 4 | 43 | 6 | 8.035 | 9.621 | 6.604 | -4.305 |
| 4 | 44 | 7 | 17.387 | 17.037 | 15.272 | 7.551 |
| 4 | 45 | 7 | 6.702 | 7.474 | 3.090 | -6.808 |
| 4 | 46 | 8 | 4.874 | 7.652 | -7.652 | 0.000 |
| 4 | 47 | 9 | 13.051 | 12.766 | 12.766 | 0.000 |
| 4 | 48 | 9 | 16.189 | 15.362 | 10.158 | 11.526 |
| 4 | 49 | 10 | 12.960 | 14.258 | -1.291 | -14.200 |
| 4 | 50 | 10 | 17.267 | 16.844 | -0.218 | 16.843 |
| 4 | 51 | 11 | 14.470 | 14.447 | 0.369 | -14.442 |
| 4 | 52 | 11 | 4.942 | 4.676 | 4.676 | 0.000 |

SYNLEUCITE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|---|---|--------|---------|---------|---------|
| 5 | 0 | 4 | 17.804 | 19.725 | 0.000 | -19.725 |
| 5 | 0 | 5 | 7.019 | 6.707 | 0.000 | -5.707 |
| 5 | 0 | 6 | 21.313 | 21.203 | 0.000 | -21.203 |
| 5 | 0 | 7 | 9.613 | 8.112 | 0.000 | -8.112 |
| 5 | 0 | 8 | 7.967 | 8.711 | 0.000 | 8.711 |
| 5 | 0 | 9 | 15.701 | 14.032 | 0.000 | -14.032 |
| 5 | 1 | 0 | 7.763 | 8.949 | 0.000 | 8.949 |
| 5 | 1 | 1 | 50.065 | 48.067 | -48.067 | 0.000 |
| 5 | 1 | 2 | 44.618 | 44.061 | 3.164 | -43.950 |
| 5 | 1 | 3 | 13.256 | 13.734 | 5.397 | -12.851 |
| 5 | 1 | 4 | 48.586 | 47.659 | 15.749 | -44.964 |
| 5 | 1 | 5 | 37.480 | 36.597 | 38.721 | 7.455 |
| 5 | 1 | 6 | 18.906 | 18.119 | 8.745 | 16.817 |
| 5 | 1 | 7 | 6.028 | 6.346 | 6.232 | 0.398 |
| 5 | 1 | 8 | 20.144 | 20.050 | 7.374 | 18.645 |
| 5 | 1 | 9 | 16.843 | 16.007 | 11.843 | -10.985 |
| 5 | 2 | 0 | 10.679 | 9.290 | -9.290 | 0.000 |
| 5 | 2 | 1 | 8.007 | 8.871 | -8.284 | -3.171 |
| 5 | 2 | 2 | 6.543 | 4.764 | -4.352 | -2.127 |
| 5 | 2 | 3 | 24.326 | 24.196 | 23.979 | -3.232 |
| 5 | 2 | 4 | 12.297 | 11.420 | -6.746 | -9.215 |
| 5 | 2 | 5 | 11.247 | 12.548 | 11.091 | -5.887 |
| 5 | 2 | 6 | 8.228 | 8.860 | -3.503 | -8.128 |
| 5 | 2 | 7 | 12.597 | 12.172 | -10.779 | -5.653 |
| 5 | 2 | 8 | 5.306 | 6.240 | 5.900 | -2.032 |
| 5 | 2 | 9 | 42.167 | 42.893 | 42.893 | 0.000 |
| 5 | 3 | 0 | 47.541 | 47.275 | -1.771 | 47.242 |
| 5 | 3 | 1 | 23.430 | 23.127 | 22.951 | 2.854 |
| 5 | 3 | 2 | 28.849 | 28.330 | -28.319 | -0.783 |
| 5 | 3 | 3 | 23.021 | 23.011 | 22.095 | 6.427 |
| 5 | 3 | 4 | 33.065 | 32.749 | 8.894 | -31.574 |
| 5 | 3 | 5 | 5.833 | 6.252 | 3.763 | 4.993 |
| 5 | 3 | 6 | 23.691 | 25.240 | 24.911 | -4.065 |
| 5 | 3 | 7 | 23.294 | 23.802 | 23.802 | 0.000 |
| 5 | 4 | 0 | 20.734 | 22.546 | -19.986 | 10.435 |
| 5 | 4 | 1 | 42.808 | 41.800 | 10.269 | -40.519 |
| 5 | 4 | 2 | 12.217 | 13.511 | 6.846 | 11.648 |
| 5 | 4 | 3 | 15.230 | 14.086 | -7.264 | -12.058 |
| 5 | 4 | 4 | 7.740 | 9.115 | 6.922 | -9.931 |
| 5 | 4 | 5 | 8.370 | 10.061 | -3.347 | 9.488 |
| 5 | 4 | 6 | 6.423 | 8.870 | -3.968 | -7.938 |
| 5 | 4 | 7 | 5.249 | 4.377 | 3.502 | -2.486 |
| 5 | 5 | 0 | 14.078 | 14.533 | -14.533 | 0.000 |
| 5 | 5 | 1 | 26.358 | 27.637 | 27.614 | 1.143 |
| 5 | 5 | 2 | 47.654 | 46.774 | -5.363 | -46.465 |
| 5 | 5 | 3 | 7.115 | 6.061 | -0.101 | 6.061 |
| 5 | 5 | 4 | 13.182 | 13.273 | 12.966 | -2.839 |
| 5 | 5 | 5 | 6.338 | 6.651 | 5.370 | 3.925 |
| 5 | 5 | 6 | 30.012 | 29.021 | 14.423 | 25.183 |
| 5 | 5 | 7 | 10.015 | 12.413 | 12.411 | -0.250 |
| 5 | 6 | 0 | 22.460 | 21.584 | -21.584 | 0.000 |
| 5 | 6 | 1 | 19.316 | 20.851 | 20.526 | -3.564 |
| 5 | 6 | 2 | 11.452 | 10.436 | -9.572 | 9.060 |

GYNNEUITE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|----|---|--------|---------|---------|---------|
| 5 | 6 | 3 | 5.774 | 6.200 | -5.228 | -3.333 |
| 5 | 6 | 4 | 17.545 | 17.132 | 11.418 | -12.772 |
| 5 | 6 | 5 | 9.913 | 10.181 | -7.525 | 6.857 |
| 5 | 6 | 6 | 21.018 | 20.499 | 2.866 | -20.298 |
| 5 | 6 | 7 | 9.432 | 8.278 | 2.920 | 7.746 |
| 5 | 6 | 8 | 5.566 | 6.534 | -5.376 | -3.714 |
| 5 | 7 | 0 | 4.256 | 4.591 | -4.591 | 0.000 |
| 5 | 7 | 1 | 39.805 | 39.395 | 36.593 | 16.866 |
| 5 | 7 | 2 | 6.741 | 6.254 | -6.788 | -9.369 |
| 5 | 7 | 3 | 16.359 | 15.949 | -1.735 | 15.864 |
| 5 | 7 | 4 | 4.857 | 6.080 | 1.863 | 5.781 |
| 5 | 7 | 5 | 13.755 | 14.322 | -3.711 | -13.833 |
| 5 | 7 | 6 | 13.716 | 12.514 | 10.379 | 6.991 |
| 5 | 7 | 7 | 18.970 | 19.267 | 13.255 | -13.901 |
| 5 | 7 | 8 | 9.049 | 8.909 | -8.909 | 0.000 |
| 5 | 8 | 0 | 17.994 | 17.189 | 17.100 | 1.721 |
| 5 | 8 | 1 | 15.781 | 14.289 | -14.172 | 1.828 |
| 5 | 8 | 2 | 15.956 | 15.660 | 10.145 | -11.926 |
| 5 | 8 | 3 | 13.426 | 12.445 | -11.986 | 3.349 |
| 5 | 8 | 4 | 14.385 | 15.807 | 2.931 | -15.529 |
| 5 | 8 | 5 | 8.001 | 9.362 | 7.473 | 5.613 |
| 5 | 8 | 6 | 7.289 | 7.860 | -7.860 | 0.000 |
| 5 | 8 | 7 | 9.539 | 9.932 | 1.654 | -9.793 |
| 5 | 8 | 8 | 27.720 | 26.994 | 24.766 | -7.895 |
| 5 | 9 | 0 | 21.455 | 21.011 | 17.800 | 11.164 |
| 5 | 9 | 1 | 5.408 | 6.309 | 4.026 | -4.858 |
| 5 | 9 | 2 | 9.210 | 11.037 | -3.936 | 10.311 |
| 5 | 9 | 3 | 10.925 | 14.861 | 14.861 | 0.000 |
| 5 | 9 | 4 | 19.700 | 19.394 | -13.716 | 13.711 |
| 5 | 9 | 5 | 22.721 | 22.765 | 4.285 | -22.562 |
| 5 | 9 | 6 | 20.547 | 17.998 | 8.238 | 16.002 |
| 5 | 9 | 7 | 11.559 | 12.519 | -7.057 | -10.340 |
| 5 | 9 | 8 | 7.343 | 8.740 | 8.546 | -1.830 |
| 5 | 10 | 1 | 7.661 | 10.463 | 10.462 | 0.162 |
| 5 | 10 | 2 | 15.497 | 16.542 | -1.330 | 16.509 |
| 5 | 10 | 3 | 12.881 | 12.488 | 12.519 | -2.063 |
| 5 | 10 | 4 | 6.429 | 6.645 | 5.997 | -2.861 |
| 5 | 10 | 5 | 12.404 | 12.223 | 12.223 | 0.000 |
| 5 | 10 | 6 | 7.774 | 8.205 | -5.854 | -5.748 |
| 5 | 10 | 7 | 8.069 | 7.490 | 7.219 | -1.998 |
| 5 | 10 | 8 | 10.685 | 11.607 | -10.836 | -4.160 |
| 5 | 10 | 9 | 10.044 | 11.983 | -11.983 | 0.000 |
| 5 | 10 | 0 | 12.245 | 13.503 | 13.458 | -1.099 |
| 5 | 0 | 1 | 24.758 | 24.439 | 24.439 | 0.000 |
| 5 | 0 | 2 | 39.812 | 38.785 | -38.785 | 0.000 |
| 5 | 0 | 3 | 42.029 | 41.636 | 41.536 | 0.000 |
| 5 | 0 | 4 | 42.099 | 40.973 | 40.973 | 0.000 |
| 5 | 0 | 5 | 33.513 | 32.539 | 32.539 | 0.000 |
| 5 | 0 | 6 | 31.199 | 31.381 | 31.381 | 0.000 |
| 5 | 0 | 7 | 6.588 | 8.104 | -8.104 | 0.000 |
| 5 | 1 | 0 | 7.144 | 8.129 | -8.129 | 0.000 |
| 5 | 1 | 1 | 22.102 | 20.542 | 10.857 | -17.438 |
| 5 | 1 | 2 | 44.909 | 44.362 | -7.275 | 43.781 |

SYNLEUCITE(4)

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|---|----|---------|---------|----------|----------|
| 6 | 1 | 3 | 24. 559 | 22. 769 | -2. 876 | -22. 586 |
| 6 | 1 | 4 | 21. 387 | 21. 279 | -2. 884 | 21. 080 |
| 6 | 1 | 5 | 6. 582 | 4. 898 | -4. 626 | 1. 609 |
| 6 | 1 | 7 | 5. 351 | 5. 149 | 0. 326 | 5. 140 |
| 6 | 0 | 6 | 68. 298 | 67. 614 | 67. 614 | 0. 000 |
| 6 | 1 | 8 | 38. 456 | 38. 802 | 10. 962 | -37. 224 |
| 6 | 2 | 6 | 62. 992 | 60. 486 | 38. 360 | 44. 332 |
| 6 | 3 | 3 | 37. 293 | 36. 390 | -0. 615 | -36. 385 |
| 6 | 4 | 4 | 11. 877 | 11. 442 | 2. 926 | 11. 061 |
| 6 | 5 | 5 | 13. 953 | 13. 437 | 1. 466 | 13. 417 |
| 6 | 6 | 6 | 21. 461 | 20. 759 | 2. 890 | -20. 557 |
| 6 | 7 | 7 | 14. 884 | 15. 847 | 11. 467 | 10. 938 |
| 6 | 8 | 8 | 9. 471 | 9. 410 | 9. 239 | -1. 787 |
| 6 | 0 | 10 | 10. 600 | 10. 866 | -10. 866 | 0. 000 |
| 6 | 1 | 11 | 21. 092 | 22. 126 | -19. 547 | 10. 367 |
| 6 | 2 | 12 | 13. 976 | 15. 702 | 8. 591 | -13. 143 |
| 6 | 3 | 13 | 10. 969 | 10. 412 | 4. 282 | 9. 491 |
| 6 | 4 | 14 | 20. 127 | 20. 341 | 13. 433 | 15. 274 |
| 6 | 5 | 15 | 12. 546 | 12. 034 | 3. 018 | -11. 650 |
| 6 | 6 | 16 | 25. 382 | 26. 157 | -4. 094 | 25. 835 |
| 6 | 7 | 17 | 10. 549 | 12. 825 | -3. 748 | -12. 265 |
| 6 | 8 | 18 | 17. 035 | 16. 798 | 16. 798 | 0. 000 |
| 6 | 0 | 19 | 7. 359 | 9. 283 | 6. 940 | 2. 499 |
| 6 | 1 | 20 | 47. 433 | 47. 495 | 26. 113 | -39. 672 |
| 6 | 2 | 21 | 4. 920 | 6. 306 | 0. 845 | 6. 249 |
| 6 | 3 | 22 | 35. 080 | 33. 122 | 32. 955 | -3. 326 |
| 6 | 4 | 23 | 5. 847 | 7. 853 | 7. 625 | 1. 878 |
| 6 | 5 | 24 | 18. 987 | 20. 243 | 11. 246 | 16. 831 |
| 6 | 6 | 25 | 10. 248 | 10. 866 | 10. 490 | -2. 834 |
| 6 | 7 | 26 | 7. 632 | 8. 822 | -8. 689 | -1. 530 |
| 6 | 8 | 27 | 22. 323 | 21. 584 | 21. 584 | 0. 000 |
| 6 | 0 | 28 | 19. 305 | 20. 851 | -20. 525 | 3. 644 |
| 6 | 1 | 29 | 11. 315 | 10. 636 | 5. 572 | -9. 060 |
| 6 | 2 | 30 | 5. 589 | 6. 200 | 5. 226 | 3. 333 |
| 6 | 3 | 31 | 18. 045 | 17. 132 | -11. 418 | 12. 772 |
| 6 | 4 | 32 | 8. 387 | 10. 181 | 7. 525 | -6. 957 |
| 6 | 5 | 33 | 22. 369 | 20. 499 | -2. 865 | 20. 298 |
| 6 | 6 | 34 | 8. 614 | 9. 278 | -2. 920 | -7. 746 |
| 6 | 7 | 35 | 4. 681 | 6. 534 | 5. 376 | 3. 714 |
| 6 | 8 | 36 | 32. 174 | 33. 499 | 33. 499 | 0. 000 |
| 6 | 0 | 37 | 31. 725 | 33. 151 | 30. 886 | 12. 043 |
| 6 | 1 | 38 | 19. 412 | 19. 964 | 19. 928 | -1. 187 |
| 6 | 2 | 39 | 16. 201 | 15. 838 | -13. 540 | 8. 217 |
| 6 | 3 | 40 | 10. 095 | 9. 615 | 7. 851 | 5. 554 |
| 6 | 4 | 41 | 20. 621 | 19. 998 | -9. 191 | -17. 761 |
| 6 | 5 | 42 | 12. 070 | 11. 567 | 8. 168 | 8. 190 |
| 6 | 6 | 43 | 22. 891 | 22. 662 | 16. 859 | -15. 144 |
| 6 | 7 | 44 | 17. 455 | 15. 822 | -15. 822 | 0. 000 |
| 6 | 8 | 45 | 10. 543 | 11. 828 | 11. 363 | -3. 284 |
| 6 | 0 | 46 | 23. 237 | 21. 212 | -4. 422 | 20. 746 |
| 6 | 1 | 47 | 9. 448 | 10. 154 | -8. 442 | -5. 641 |
| 6 | 2 | 48 | 12. 569 | 10. 787 | 8. 361 | 6. 215 |
| 6 | 3 | 49 | 5. 646 | 7. 569 | -7. 567 | -0. 156 |

SYNLEUCATE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|----|---|---------|---------|----------|----------|
| 6 | 7 | 6 | 5. 856 | 4. 795 | 2. 428 | -4. 093 |
| 6 | 7 | 7 | 5. 657 | 5. 481 | 4. 685 | 2. 894 |
| 6 | 8 | 0 | 18. 130 | 17. 190 | 17. 190 | 0. 000 |
| 6 | 8 | 1 | 13. 488 | 15. 486 | -12. 147 | -9. 468 |
| 6 | 8 | 2 | 18. 136 | 17. 271 | 18. 654 | 4. 568 |
| 6 | 8 | 3 | 25. 166 | 24. 550 | 21. 511 | -11. 832 |
| 6 | 8 | 4 | 10. 237 | 10. 674 | 10. 663 | -0. 473 |
| 6 | 8 | 5 | 20. 062 | 19. 133 | 18. 778 | 3. 669 |
| 6 | 9 | 1 | 6. 554 | 7. 042 | 4. 989 | -6. 068 |
| 6 | 9 | 2 | 14. 561 | 14. 714 | 1. 826 | 14. 599 |
| 6 | 9 | 3 | 15. 762 | 14. 448 | -12. 799 | -6. 703 |
| 6 | 9 | 4 | 7. 751 | 9. 978 | 9. 290 | 3. 643 |
| 6 | 9 | 5 | 7. 502 | 7. 652 | -7. 379 | 2. 027 |
| 6 | 10 | 0 | 28. 389 | 26. 761 | 26. 761 | 0. 000 |
| 6 | 10 | 1 | 17. 699 | 16. 882 | 12. 089 | 11. 784 |
| 6 | 10 | 2 | 12. 858 | 12. 368 | 11. 795 | 3. 721 |
| 6 | 10 | 3 | 4. 903 | 5. 657 | -5. 220 | -4. 132 |
| 6 | 10 | 4 | 7. 785 | 9. 295 | 9. 170 | -1. 514 |
| 6 | 10 | 5 | 9. 474 | 10. 716 | 0. 892 | -10. 479 |
| 6 | 11 | 0 | 20. 672 | 19. 747 | 18. 747 | 0. 000 |
| 6 | 11 | 1 | 9. 607 | 10. 087 | -9. 935 | 1. 744 |
| 6 | 11 | 2 | 10. 362 | 10. 774 | 10. 702 | 1. 243 |
| 6 | 11 | 3 | 21. 574 | 19. 562 | -19. 322 | 3. 053 |
| 6 | 11 | 4 | 10. 095 | 10. 612 | 10. 368 | -2. 264 |
| 6 | 12 | 0 | 4. 852 | 4. 755 | -4. 755 | 0. 000 |
| 6 | 12 | 1 | 5. 289 | 3. 191 | 3. 179 | 0. 428 |
| 6 | 12 | 2 | 7. 036 | 9. 619 | 6. 617 | -6. 991 |
| 6 | 12 | 3 | 15. 662 | 15. 881 | 15. 879 | -0. 276 |
| 6 | 13 | 2 | 5. 941 | 8. 063 | -2. 353 | -7. 712 |
| 7 | 0 | 2 | 27. 340 | 27. 695 | 0. 000 | 27. 695 |
| 7 | 0 | 3 | 4. 715 | 2. 792 | 0. 000 | -2. 792 |
| 7 | 0 | 4 | 15. 247 | 15. 947 | 0. 000 | -15. 947 |
| 7 | 0 | 5 | 28. 491 | 29. 680 | 0. 000 | -29. 680 |
| 7 | 0 | 6 | 6. 395 | 7. 352 | 0. 000 | 7. 352 |
| 7 | 1 | 0 | 8. 393 | 8. 948 | 8. 948 | 0. 000 |
| 7 | 1 | 1 | 5. 453 | 5. 311 | 4. 338 | -3. 064 |
| 7 | 1 | 2 | 22. 806 | 22. 604 | -6. 761 | 21. 569 |
| 7 | 1 | 3 | 34. 376 | 34. 001 | 33. 665 | -4. 764 |
| 7 | 1 | 4 | 20. 320 | 19. 525 | -16. 142 | 10. 984 |
| 7 | 1 | 5 | 23. 572 | 23. 251 | 22. 698 | -5. 037 |
| 7 | 1 | 6 | 8. 654 | 8. 744 | 6. 687 | -5. 634 |
| 7 | 1 | 7 | 20. 298 | 20. 364 | 20. 339 | -0. 459 |
| 7 | 2 | 0 | 37. 400 | 39. 548 | -39. 548 | 0. 000 |
| 7 | 2 | 1 | 25. 149 | 24. 352 | 24. 266 | 1. 759 |
| 7 | 2 | 2 | 18. 056 | 18. 211 | -0. 906 | -18. 289 |
| 7 | 2 | 3 | 17. 818 | 16. 002 | -15. 395 | 4. 364 |
| 7 | 2 | 4 | 34. 325 | 33. 740 | 29. 450 | -16. 465 |
| 7 | 2 | 5 | 20. 752 | 19. 981 | -16. 337 | 7. 938 |
| 7 | 2 | 6 | 8. 983 | 9. 274 | 2. 049 | -9. 045 |
| 7 | 2 | 7 | 7. 882 | 9. 710 | 7. 408 | 6. 277 |
| 7 | 2 | 8 | 15. 037 | 15. 275 | -14. 323 | -5. 307 |
| 7 | 3 | 0 | 37. 207 | 37. 082 | -37. 082 | 0. 000 |
| 7 | 3 | 1 | 40. 635 | 40. 052 | 33. 982 | -21. 179 |

SYNTHETIC

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|----|---|--------|---------|---------|---------|
| 7 | 3 | 2 | 22.267 | 22.927 | -4.828 | -22.413 |
| 7 | 3 | 3 | 15.259 | 15.789 | -1.751 | -15.692 |
| 7 | 3 | 4 | 28.968 | 28.100 | 27.698 | 4.740 |
| 7 | 3 | 5 | 11.695 | 12.593 | -1.590 | 12.452 |
| 7 | 3 | 6 | 17.487 | 19.603 | 11.617 | 15.790 |
| 7 | 3 | 7 | 13.971 | 14.656 | 13.633 | 5.380 |
| 7 | 4 | 0 | 26.318 | 26.988 | 26.988 | 0.000 |
| 7 | 4 | 1 | 29.331 | 28.464 | -27.630 | 6.240 |
| 7 | 4 | 2 | 27.532 | 27.045 | 14.865 | -22.594 |
| 7 | 4 | 3 | 12.785 | 12.543 | 5.276 | 11.379 |
| 7 | 4 | 4 | 9.781 | 11.576 | -3.392 | -11.068 |
| 7 | 4 | 5 | 8.709 | 8.058 | 8.045 | 0.454 |
| 7 | 4 | 7 | 5.459 | 5.351 | -3.329 | -4.139 |
| 7 | 4 | 8 | 5.255 | 3.997 | 0.180 | -3.993 |
| 7 | 5 | 0 | 4.653 | 4.591 | -4.591 | 0.000 |
| 7 | 5 | 1 | 39.425 | 39.395 | 35.593 | 16.895 |
| 7 | 5 | 2 | 6.804 | 6.254 | -5.788 | -2.369 |
| 7 | 5 | 3 | 15.786 | 15.949 | -1.735 | 15.854 |
| 7 | 5 | 4 | 5.953 | 6.080 | -1.883 | 5.781 |
| 7 | 5 | 5 | 14.396 | 14.322 | -3.711 | -13.833 |
| 7 | 5 | 6 | 11.996 | 12.514 | 10.379 | 5.991 |
| 7 | 5 | 7 | 18.760 | 19.207 | 13.255 | -13.900 |
| 7 | 6 | 0 | 16.286 | 15.622 | 15.622 | 0.000 |
| 7 | 6 | 1 | 10.441 | 11.828 | -11.563 | 3.284 |
| 7 | 6 | 2 | 21.779 | 21.212 | 4.422 | -20.746 |
| 7 | 6 | 3 | 8.779 | 10.164 | 8.442 | 5.681 |
| 7 | 6 | 4 | 10.781 | 10.787 | -8.361 | -6.816 |
| 7 | 6 | 5 | 5.476 | 7.569 | 7.567 | 0.156 |
| 7 | 7 | 1 | 11.582 | 15.117 | -3.011 | -14.814 |
| 7 | 7 | 2 | 13.596 | 13.502 | 1.553 | 13.412 |
| 7 | 7 | 3 | 30.818 | 29.560 | 21.963 | -19.784 |
| 7 | 7 | 4 | 9.527 | 10.505 | 6.395 | 8.334 |
| 7 | 7 | 5 | 16.836 | 17.074 | 17.054 | 0.811 |
| 7 | 8 | 0 | 7.326 | 6.860 | 4.815 | 4.801 |
| 7 | 8 | 3 | 8.858 | 8.881 | -8.748 | -1.528 |
| 7 | 8 | 4 | 11.542 | 11.398 | 9.034 | -6.949 |
| 7 | 8 | 5 | 6.429 | 7.220 | -5.533 | 4.639 |
| 7 | 8 | 6 | 12.489 | 11.392 | 0.758 | -11.367 |
| 7 | 9 | 0 | 15.786 | 13.991 | 13.991 | 0.000 |
| 7 | 9 | 2 | 24.139 | 22.742 | 3.071 | 22.523 |
| 7 | 9 | 3 | 12.211 | 13.120 | 13.110 | 0.509 |
| 7 | 9 | 4 | 7.678 | 7.405 | -7.384 | 0.559 |
| 7 | 9 | 5 | 12.597 | 13.591 | 2.258 | -13.401 |
| 7 | 10 | 0 | 7.700 | 8.583 | 8.583 | 0.000 |
| 7 | 10 | 1 | 6.384 | 7.536 | 1.473 | -7.391 |
| 7 | 10 | 2 | 14.623 | 14.370 | 3.662 | 13.885 |
| 7 | 10 | 3 | 10.855 | 10.576 | -7.521 | -7.578 |
| 7 | 10 | 5 | 6.004 | 5.627 | -2.751 | 4.900 |
| 7 | 11 | 0 | 6.089 | 8.078 | -9.071 | 0.000 |
| 7 | 11 | 1 | 8.506 | 9.824 | 6.995 | 6.899 |
| 7 | 11 | 2 | 18.697 | 17.610 | 0.942 | -17.585 |
| 7 | 11 | 3 | 7.526 | 8.995 | 6.840 | 5.841 |
| 7 | 11 | 4 | 10.101 | 9.532 | 9.513 | 0.604 |

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|----|---|--------|---------|---------|---------|
| 7 | 12 | 0 | 4.492 | 3.701 | -3.701 | 0.000 |
| 7 | 12 | 2 | 12.495 | 13.405 | -0.901 | -13.375 |
| 7 | 12 | 3 | 7.195 | 7.437 | 3.489 | 6.568 |
| 8 | 0 | 0 | 50.684 | 47.540 | 47.540 | 0.000 |
| 8 | 0 | 1 | 15.395 | 15.651 | 15.651 | 0.000 |
| 8 | 0 | 2 | 14.129 | 14.561 | 14.561 | 0.000 |
| 8 | 0 | 3 | 16.422 | 17.125 | 17.125 | 0.000 |
| 8 | 0 | 4 | 16.144 | 15.305 | -15.305 | 0.000 |
| 8 | 0 | 5 | 12.524 | 11.539 | 11.539 | 0.000 |
| 8 | 0 | 3 | 21.257 | 19.574 | 19.574 | 0.000 |
| 8 | 1 | 0 | 41.497 | 40.816 | -40.816 | 0.000 |
| 8 | 1 | 1 | 27.044 | 27.491 | 23.451 | 14.345 |
| 8 | 1 | 2 | 4.477 | 7.705 | -6.721 | 3.768 |
| 8 | 1 | 3 | 14.765 | 14.875 | -10.239 | 10.790 |
| 8 | 1 | 4 | 23.946 | 23.867 | 23.655 | 3.174 |
| 8 | 1 | 5 | 15.503 | 14.913 | -12.259 | -8.493 |
| 8 | 1 | 6 | 5.369 | 7.571 | 2.803 | 7.032 |
| 8 | 1 | 8 | 11.094 | 12.627 | -11.560 | 5.082 |
| 8 | 2 | 0 | 14.243 | 15.161 | 15.161 | 0.000 |
| 8 | 2 | 2 | 34.711 | 33.422 | 19.577 | -27.089 |
| 8 | 2 | 3 | 12.756 | 11.773 | 11.762 | 0.523 |
| 8 | 2 | 4 | 23.958 | 21.381 | 21.122 | 3.321 |
| 8 | 2 | 5 | 10.316 | 11.712 | 11.651 | -1.196 |
| 8 | 2 | 6 | 18.907 | 19.052 | 8.227 | 17.154 |
| 8 | 2 | 7 | 5.845 | 6.594 | 4.064 | -5.193 |
| 8 | 3 | 0 | 10.662 | 11.464 | -11.464 | 0.000 |
| 8 | 3 | 1 | 19.991 | 19.468 | 14.061 | -13.465 |
| 8 | 3 | 2 | 20.672 | 20.812 | -1.553 | 20.754 |
| 8 | 3 | 3 | 18.033 | 17.686 | -14.159 | -10.597 |
| 8 | 3 | 4 | 10.265 | 10.690 | 8.971 | 5.815 |
| 8 | 3 | 5 | 17.392 | 17.088 | -12.097 | 12.069 |
| 8 | 3 | 6 | 6.724 | 9.195 | 2.197 | -8.928 |
| 8 | 3 | 7 | 12.943 | 12.646 | 7.837 | 9.928 |
| 8 | 4 | 0 | 11.655 | 13.627 | 13.627 | 0.000 |
| 8 | 4 | 1 | 31.278 | 32.069 | 31.289 | 7.031 |
| 8 | 4 | 2 | 20.439 | 19.796 | 17.626 | -9.011 |
| 8 | 4 | 3 | 16.450 | 16.482 | -11.814 | 11.493 |
| 8 | 4 | 4 | 21.149 | 18.369 | 17.587 | -5.303 |
| 8 | 4 | 5 | 7.695 | 9.764 | -9.704 | 1.075 |
| 8 | 4 | 7 | 16.819 | 16.229 | 15.815 | -3.643 |
| 8 | 5 | 0 | 7.002 | 8.909 | 8.909 | 0.000 |
| 8 | 5 | 1 | 16.933 | 17.189 | -17.103 | -1.721 |
| 8 | 5 | 3 | 14.629 | 14.289 | 14.172 | -1.828 |
| 8 | 5 | 4 | 16.711 | 15.660 | -10.149 | 11.926 |
| 8 | 5 | 5 | 10.804 | 12.445 | 11.966 | -3.349 |
| 8 | 5 | 6 | 14.532 | 15.807 | -2.951 | 15.529 |
| 8 | 5 | 7 | 9.584 | 9.362 | -7.493 | -5.613 |
| 8 | 6 | 0 | 17.494 | 17.190 | 17.190 | 0.000 |
| 8 | 6 | 1 | 13.982 | 15.486 | -12.147 | -9.805 |
| 8 | 6 | 2 | 17.931 | 17.271 | 16.636 | 4.568 |
| 8 | 6 | 3 | 24.514 | 24.550 | 21.511 | -11.832 |
| 8 | 6 | 4 | 19.556 | 10.674 | 10.663 | -0.473 |
| 8 | 6 | 5 | 18.618 | 19.133 | 18.778 | 3.669 |

SYNTHETIC CRYSTAL

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|---|----|---|--------|---------|---------|---------|
| 8 | 5 | 7 | 6.446 | 7.528 | -3.905 | 6.435 |
| 8 | 7 | 2 | 6.560 | 6.800 | -4.815 | -4.801 |
| 8 | 7 | 3 | 8.052 | 8.881 | 9.748 | 1.528 |
| 8 | 7 | 4 | 12.001 | 11.398 | -9.084 | 6.949 |
| 8 | 7 | 5 | 6.673 | 7.220 | 5.533 | -4.639 |
| 8 | 7 | 6 | 12.665 | 11.392 | -0.758 | 11.367 |
| 8 | 8 | 0 | 34.472 | 32.941 | 32.941 | 0.000 |
| 8 | 8 | 2 | 31.942 | 30.493 | 18.872 | 23.952 |
| 8 | 8 | 3 | 4.840 | 5.354 | 4.962 | -2.089 |
| 8 | 8 | 6 | 19.168 | 18.615 | 0.739 | -18.600 |
| 8 | 8 | 9 | 4.918 | 6.620 | 2.921 | -5.940 |
| 8 | 9 | 2 | 16.297 | 15.156 | -0.959 | 15.126 |
| 8 | 9 | 3 | 10.072 | 10.143 | -5.166 | -8.728 |
| 8 | 9 | 4 | 7.048 | 7.083 | 1.857 | 6.835 |
| 8 | 10 | 1 | 5.436 | 6.587 | 5.229 | 4.006 |
| 8 | 10 | 2 | 24.304 | 21.080 | 10.674 | -18.177 |
| 8 | 10 | 3 | 5.691 | 5.077 | -1.068 | 4.960 |
| 8 | 10 | 4 | 25.064 | 22.315 | 21.930 | 1.130 |
| 8 | 11 | 0 | 8.046 | 8.754 | -8.754 | 0.000 |
| 8 | 11 | 1 | 8.251 | 9.381 | 9.447 | -4.079 |
| 8 | 11 | 2 | 8.540 | 8.628 | -3.466 | 7.901 |
| 8 | 11 | 3 | 7.519 | 8.433 | -4.914 | -6.853 |
| 8 | 12 | 0 | 23.658 | 21.510 | 21.510 | 0.000 |
| 8 | 12 | 1 | 7.150 | 7.659 | 1.151 | 7.572 |
| 8 | 12 | 2 | 11.933 | 12.093 | 9.139 | -7.904 |
| 9 | 0 | 1 | 27.493 | 27.293 | 0.000 | 27.253 |
| 9 | 0 | 2 | 41.622 | 37.178 | 0.000 | -37.178 |
| 9 | 0 | 3 | 24.338 | 24.092 | 0.000 | 24.092 |
| 9 | 0 | 4 | 10.793 | 10.828 | 0.000 | -10.828 |
| 9 | 0 | 5 | 18.408 | 17.445 | 0.000 | -17.445 |
| 9 | 0 | 6 | 19.970 | 17.691 | 0.000 | 17.691 |
| 9 | 0 | 7 | 14.067 | 13.543 | 0.000 | -13.543 |
| 9 | 1 | 1 | 21.994 | 20.864 | 20.491 | -3.926 |
| 9 | 1 | 2 | 18.448 | 18.132 | -4.864 | -17.467 |
| 9 | 1 | 3 | 8.557 | 10.760 | 10.312 | -3.073 |
| 9 | 1 | 5 | 7.025 | 7.348 | 7.327 | 0.556 |
| 9 | 1 | 6 | 16.728 | 16.715 | 9.625 | 13.665 |
| 9 | 2 | 1 | 14.283 | 14.722 | 14.168 | 3.927 |
| 9 | 2 | 2 | 6.429 | 6.350 | -4.803 | 4.153 |
| 9 | 2 | 3 | 7.570 | 8.360 | -5.863 | 6.959 |
| 9 | 2 | 4 | 14.027 | 13.217 | -11.118 | -13.164 |
| 9 | 2 | 5 | 5.652 | 6.508 | -4.667 | 4.536 |
| 9 | 2 | 6 | 18.323 | 17.121 | 3.080 | -16.842 |
| 9 | 3 | 1 | 25.989 | 25.249 | 20.215 | 15.126 |
| 9 | 3 | 2 | 13.891 | 14.001 | 1.449 | -13.925 |
| 9 | 3 | 3 | 19.117 | 18.024 | 0.593 | 18.014 |
| 9 | 3 | 4 | 8.007 | 7.575 | 7.438 | -1.434 |
| 9 | 3 | 5 | 8.302 | 8.725 | 7.504 | 4.451 |
| 9 | 3 | 7 | 9.720 | 12.310 | 9.921 | -7.288 |
| 9 | 4 | 0 | 7.899 | 7.818 | 7.818 | 0.000 |
| 9 | 4 | 1 | 20.311 | 22.637 | 9.053 | -20.743 |
| 9 | 4 | 2 | 10.458 | 11.255 | 0.173 | 11.254 |
| 9 | 4 | 3 | 17.392 | 19.291 | -6.352 | -17.153 |

SYNLEUCITE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|----|----|---|--------|---------|---------|---------|
| 9 | 4 | 4 | 7.110 | 8.506 | 7.377 | -4.235 |
| 9 | 4 | 5 | 18.595 | 18.395 | -5.131 | 17.665 |
| 9 | 4 | 6 | 17.449 | 17.102 | 1.214 | -17.059 |
| 9 | 4 | 7 | 12.058 | 14.037 | 13.318 | 13.640 |
| 9 | 5 | 0 | 8.705 | 7.860 | -7.860 | 0.000 |
| 9 | 5 | 1 | 8.404 | 9.922 | 1.454 | -9.793 |
| 9 | 5 | 3 | 26.910 | 25.994 | 24.756 | -7.895 |
| 9 | 5 | 5 | 20.927 | 21.011 | 17.801 | 11.164 |
| 9 | 5 | 7 | 7.910 | 11.037 | -3.936 | 10.311 |
| 9 | 6 | 1 | 6.162 | 7.042 | -4.889 | 5.068 |
| 9 | 6 | 2 | 12.689 | 14.714 | -1.836 | -14.599 |
| 9 | 6 | 3 | 16.002 | 14.448 | 12.799 | 6.703 |
| 9 | 6 | 4 | 9.147 | 9.978 | -9.290 | -3.643 |
| 9 | 6 | 5 | 7.462 | 7.652 | 7.379 | -2.027 |
| 9 | 7 | 0 | 14.010 | 13.991 | 13.991 | 0.000 |
| 9 | 7 | 2 | 23.311 | 22.742 | 13.071 | 22.533 |
| 9 | 7 | 3 | 12.745 | 13.120 | 13.110 | 0.509 |
| 9 | 7 | 4 | 5.987 | 7.405 | -7.394 | 0.559 |
| 9 | 7 | 5 | 8.089 | 8.227 | 8.155 | -1.091 |
| 9 | 7 | 6 | 13.613 | 13.591 | 2.260 | -13.401 |
| 9 | 8 | 2 | 15.395 | 15.156 | 0.958 | -15.126 |
| 9 | 8 | 3 | 10.061 | 10.143 | 5.166 | 5.728 |
| 9 | 8 | 4 | 8.183 | 7.083 | -1.857 | -6.936 |
| 9 | 9 | 0 | 23.668 | 22.439 | -22.439 | 0.000 |
| 9 | 9 | 1 | 14.827 | 14.717 | 14.586 | 1.962 |
| 9 | 9 | 2 | 14.861 | 14.985 | 0.687 | -14.969 |
| 9 | 9 | 4 | 25.007 | 21.694 | 21.633 | -1.625 |
| 9 | 11 | 1 | 14.504 | 15.908 | 15.791 | 1.925 |
| 10 | 0 | 0 | 18.198 | 17.186 | 17.186 | 0.000 |
| 10 | 0 | 1 | 6.378 | 6.820 | 6.820 | 0.000 |
| 10 | 0 | 2 | 14.402 | 14.357 | 14.357 | 0.000 |
| 10 | 0 | 4 | 11.150 | 12.029 | 12.029 | 0.000 |
| 10 | 0 | 5 | 7.456 | 7.576 | 7.576 | 0.000 |
| 10 | 1 | 0 | 20.621 | 19.635 | 19.635 | 0.000 |
| 10 | 1 | 1 | 8.688 | 10.391 | -1.744 | 10.243 |
| 10 | 1 | 2 | 5.930 | 6.250 | -3.079 | -5.439 |
| 10 | 1 | 3 | 6.242 | 6.350 | 3.293 | 5.430 |
| 10 | 1 | 4 | 21.427 | 20.817 | -18.661 | 9.227 |
| 10 | 1 | 5 | 17.574 | 16.414 | 5.298 | -15.535 |
| 10 | 1 | 6 | 18.584 | 17.949 | 1.186 | 17.910 |
| 10 | 1 | 7 | 10.827 | 11.648 | -0.892 | -11.613 |
| 10 | 2 | 0 | 24.593 | 24.514 | 24.514 | 0.000 |
| 10 | 2 | 1 | 12.711 | 12.810 | 9.529 | 8.094 |
| 10 | 2 | 2 | 25.229 | 23.315 | 21.253 | -9.588 |
| 10 | 2 | 3 | 15.043 | 12.900 | -9.836 | 8.346 |
| 10 | 2 | 4 | 14.135 | 13.407 | 13.386 | -0.755 |
| 10 | 2 | 5 | 5.073 | 6.395 | -3.972 | -5.012 |
| 10 | 2 | 6 | 6.128 | 6.652 | 4.655 | 4.752 |
| 10 | 2 | 7 | 14.572 | 13.665 | 12.617 | -5.247 |
| 10 | 3 | 0 | 6.270 | 6.981 | 6.981 | 0.000 |
| 10 | 3 | 1 | 8.557 | 10.762 | -0.699 | -10.739 |
| 10 | 3 | 2 | 18.936 | 17.377 | -3.234 | 17.073 |
| 10 | 3 | 3 | 11.553 | 11.556 | 0.738 | -11.532 |

SYNLEUC-TE 4

| | H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|--|----|----|---|--------|---------|---------|---------|
| | 10 | 3 | 4 | 7.995 | 10.307 | -8.083 | 6.395 |
| | 10 | 3 | 5 | 4.846 | 6.824 | 4.067 | 5.480 |
| | 10 | 3 | 6 | 4.795 | 5.479 | 1.793 | -5.178 |
| | 10 | 4 | 0 | 20.587 | 19.480 | 19.480 | 0.000 |
| | 10 | 4 | 1 | 12.762 | 13.617 | -12.073 | -6.298 |
| | 10 | 4 | 2 | 16.950 | 16.370 | 16.214 | 2.257 |
| | 10 | 4 | 3 | 18.873 | 17.232 | 16.375 | -5.367 |
| | 10 | 4 | 4 | 9.300 | 9.621 | 8.604 | -4.305 |
| | 10 | 4 | 5 | 17.835 | 17.037 | 15.272 | 7.551 |
| | 10 | 4 | 6 | 5.833 | 7.474 | 3.090 | -6.808 |
| | 10 | 5 | 0 | 14.527 | 14.861 | -14.661 | 0.000 |
| | 10 | 5 | 1 | 21.132 | 19.394 | 13.716 | -13.711 |
| | 10 | 5 | 2 | 24.009 | 22.965 | -4.285 | 22.562 |
| | 10 | 5 | 3 | 18.981 | 17.998 | -8.238 | -16.002 |
| | 10 | 5 | 4 | 13.136 | 12.519 | 7.007 | 10.340 |
| | 10 | 5 | 5 | 7.405 | 8.740 | -8.546 | 1.830 |
| | 10 | 6 | 0 | 26.244 | 26.761 | 26.761 | 0.000 |
| | 10 | 6 | 2 | 16.189 | 16.882 | 12.044 | 11.784 |
| | 10 | 6 | 3 | 13.656 | 12.368 | 11.795 | 3.721 |
| | 10 | 6 | 4 | 6.809 | 6.657 | -5.220 | -4.132 |
| | 10 | 6 | 5 | 9.046 | 9.295 | 9.170 | -1.514 |
| | 10 | 6 | 6 | 10.390 | 10.716 | 0.852 | -10.678 |
| | 10 | 7 | 0 | 7.042 | 8.583 | -8.593 | 0.000 |
| | 10 | 7 | 1 | 5.430 | 7.536 | -1.472 | 7.391 |
| | 10 | 7 | 2 | 12.331 | 14.370 | -3.662 | -13.895 |
| | 10 | 7 | 3 | 10.933 | 10.576 | 7.521 | 7.578 |
| | 10 | 7 | 5 | 6.043 | 5.627 | 2.766 | -4.500 |
| | 10 | 8 | 1 | 5.992 | 6.587 | 5.229 | 4.606 |
| | 10 | 8 | 2 | 22.948 | 21.080 | 10.676 | -18.177 |
| | 10 | 8 | 4 | 21.892 | 22.315 | 21.930 | -4.130 |
| | 10 | 9 | 0 | 3.966 | 2.156 | 2.156 | 0.000 |
| | 10 | 9 | 3 | 6.304 | 5.306 | 4.785 | 2.361 |
| | 10 | 9 | 4 | 5.340 | 4.853 | -4.614 | 1.505 |
| | 10 | 10 | 1 | 16.127 | 15.343 | 15.334 | 0.550 |
| | 11 | 0 | 5 | 5.425 | 5.650 | 0.000 | -5.650 |
| | 11 | 0 | 6 | 4.784 | 4.244 | 0.000 | 4.244 |
| | 11 | 1 | 1 | 20.509 | 18.799 | 17.067 | 7.878 |
| | 11 | 1 | 3 | 5.896 | 7.133 | 1.210 | 7.030 |
| | 11 | 1 | 4 | 6.009 | 6.370 | 6.263 | 1.165 |
| | 11 | 1 | 6 | 5.062 | 5.589 | 6.069 | 2.565 |
| | 11 | 2 | 0 | 35.443 | 32.154 | 32.154 | 0.000 |
| | 11 | 2 | 1 | 16.575 | 15.446 | -15.401 | -1.186 |
| | 11 | 2 | 2 | 7.632 | 7.916 | 1.581 | -7.756 |
| | 11 | 2 | 3 | 6.599 | 9.151 | 9.119 | 0.769 |
| | 11 | 2 | 4 | 23.685 | 23.614 | -23.048 | -5.137 |
| | 11 | 2 | 5 | 14.107 | 14.123 | 13.397 | 4.469 |
| | 11 | 3 | 1 | 8.875 | 8.581 | -2.800 | -8.112 |
| | 11 | 3 | 2 | 11.179 | 10.556 | 5.584 | 8.958 |
| | 11 | 3 | 3 | 15.053 | 15.404 | 12.219 | -9.379 |
| | 11 | 3 | 5 | 10.481 | 11.309 | 10.828 | 3.264 |
| | 11 | 4 | 0 | 4.914 | 7.652 | 7.652 | 0.000 |
| | 11 | 4 | 2 | 4.534 | 5.412 | 2.020 | 5.021 |
| | 11 | 5 | 1 | 9.647 | 10.463 | 10.462 | 0.162 |

SYNLEUCITE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|----|---|---|--------|---------|---------|---------|
| 11 | 5 | 2 | 15.945 | 16.562 | -1.930 | 16.509 |
| 11 | 5 | 3 | 10.713 | 12.688 | 12.519 | -2.063 |
| 11 | 5 | 5 | 5.629 | 6.645 | 5.997 | -2.851 |
| 11 | 5 | 0 | 16.762 | 18.747 | -19.747 | 0.000 |
| 11 | 6 | 1 | 10.118 | 10.087 | 9.935 | -1.744 |
| 11 | 6 | 3 | 11.535 | 10.774 | -10.702 | -1.243 |
| 11 | 6 | 4 | 19.923 | 19.562 | 19.382 | -3.053 |
| 11 | 6 | 5 | 11.757 | 10.612 | -10.358 | 2.264 |
| 11 | 7 | 0 | 6.730 | 8.078 | -8.078 | 0.000 |
| 11 | 7 | 1 | 10.736 | 9.824 | 6.995 | 6.899 |
| 11 | 7 | 2 | 17.999 | 17.610 | 9.942 | -17.585 |
| 11 | 7 | 3 | 9.011 | 8.995 | 6.840 | 5.841 |
| 11 | 7 | 4 | 8.018 | 9.632 | 9.613 | 0.604 |
| 11 | 8 | 0 | 7.456 | 9.754 | 8.754 | 0.000 |
| 11 | 8 | 1 | 10.441 | 9.381 | -9.448 | 4.079 |
| 11 | 8 | 2 | 8.620 | 9.628 | 9.466 | -7.901 |
| 11 | 8 | 3 | 8.149 | 8.433 | 4.914 | 6.853 |
| 11 | 8 | 9 | 15.310 | 15.908 | 15.791 | 1.925 |
| 12 | 0 | 0 | 15.372 | 14.329 | 14.339 | 0.000 |
| 12 | 0 | 2 | 7.780 | 7.840 | 7.840 | 0.000 |
| 12 | 0 | 4 | 8.041 | 8.549 | 8.549 | 0.000 |
| 12 | 1 | 0 | 19.112 | 17.677 | 17.577 | 0.000 |
| 12 | 1 | 1 | 20.241 | 17.814 | -19.572 | -11.536 |
| 12 | 1 | 2 | 6.514 | 8.314 | 1.364 | 6.202 |
| 12 | 1 | 3 | 14.975 | 14.393 | 8.553 | -11.576 |
| 12 | 1 | 4 | 15.208 | 14.708 | -12.634 | 7.531 |
| 12 | 1 | 5 | 9.527 | 11.180 | 10.140 | 4.708 |
| 12 | 2 | 0 | 21.295 | 18.587 | 18.587 | 0.000 |
| 12 | 2 | 1 | 7.354 | 7.226 | -5.679 | -2.759 |
| 12 | 2 | 2 | 14.158 | 13.956 | 12.878 | 5.379 |
| 12 | 2 | 3 | 8.427 | 9.998 | 9.298 | -3.480 |
| 12 | 2 | 4 | 7.814 | 9.486 | 9.457 | 0.729 |
| 12 | 2 | 5 | 16.706 | 15.418 | 15.418 | 0.000 |
| 12 | 2 | 6 | 7.269 | 9.561 | -4.946 | 8.182 |
| 12 | 2 | 7 | 6.764 | 8.038 | 0.906 | 7.985 |
| 12 | 3 | 4 | 12.552 | 11.479 | -11.479 | -0.042 |
| 12 | 3 | 0 | 13.063 | 12.766 | 12.766 | 0.000 |
| 12 | 4 | 2 | 16.728 | 15.362 | 10.136 | 11.526 |
| 12 | 5 | 0 | 12.716 | 12.223 | -12.223 | 0.000 |
| 12 | 5 | 1 | 5.334 | 8.205 | 5.854 | 5.748 |
| 12 | 5 | 3 | 6.667 | 7.490 | -7.219 | 1.996 |
| 12 | 5 | 4 | 12.751 | 11.607 | 10.835 | 4.160 |
| 12 | 6 | 1 | 7.729 | 8.190 | 8.179 | 0.428 |
| 12 | 6 | 2 | 8.761 | 9.519 | 6.617 | -6.981 |
| 12 | 6 | 4 | 16.836 | 15.881 | 15.879 | -0.277 |
| 12 | 7 | 1 | 5.300 | 5.857 | 1.241 | -5.724 |
| 12 | 7 | 2 | 11.871 | 13.405 | 0.901 | 13.375 |
| 12 | 7 | 3 | 7.558 | 7.437 | -3.489 | -6.568 |
| 12 | 8 | 0 | 21.972 | 21.510 | 21.510 | 0.000 |
| 12 | 8 | 2 | 10.208 | 12.083 | 9.139 | -7.904 |
| 13 | 0 | 1 | 26.205 | 21.554 | 0.000 | -21.554 |
| 13 | 0 | 2 | 15.202 | 14.150 | 0.000 | 14.150 |
| 13 | 0 | 3 | 19.899 | 17.993 | 0.000 | -17.993 |

SYNLEUCITE 4

| H | K | L | F(OBS) | F(CALC) | A(CALC) | B(CALC) |
|----|---|---|--------|---------|---------|---------|
| 13 | 1 | 1 | 10.231 | 9.397 | 9.137 | -2.194 |
| 13 | 1 | 3 | 11.933 | 11.212 | 11.109 | -1.517 |
| 13 | 2 | 1 | 5.022 | 5.481 | -2.930 | 4.632 |
| 13 | 2 | 2 | 9.136 | 9.508 | 1.462 | -9.395 |
| 13 | 2 | 3 | 8.546 | 8.113 | 0.418 | 8.102 |
| 13 | 2 | 4 | 6.100 | 6.650 | -1.565 | -6.463 |
| 13 | 3 | 1 | 5.277 | 5.152 | 5.761 | 2.157 |
| 13 | 3 | 3 | 5.152 | 7.849 | 7.748 | 1.258 |
| 13 | 4 | 1 | 14.521 | 14.258 | 1.291 | 14.200 |
| 13 | 4 | 2 | 19.333 | 16.844 | 0.218 | -16.843 |
| 13 | 4 | 3 | 16.484 | 14.447 | -0.369 | 14.442 |
| 13 | 5 | 0 | 8.767 | 11.983 | -11.983 | 0.000 |
| 13 | 5 | 1 | 13.732 | 13.503 | 13.468 | -1.099 |
| 13 | 6 | 2 | 6.565 | 8.063 | 2.353 | 7.712 |
| 14 | 0 | 3 | 6.441 | 6.238 | 6.298 | 0.000 |
| 14 | 1 | 0 | 11.848 | 11.926 | -11.926 | 0.000 |
| 14 | 1 | 1 | 13.029 | 11.627 | 7.813 | -9.039 |
| 14 | 1 | 2 | 5.862 | 7.548 | 0.462 | 7.554 |
| 14 | 1 | 3 | 11.281 | 11.046 | -7.140 | -8.428 |
| 14 | 2 | 0 | 10.112 | 10.728 | 10.708 | 0.000 |
| 14 | 2 | 2 | 6.065 | 8.449 | 8.193 | -2.323 |
| 14 | 3 | 0 | 13.460 | 12.740 | -12.740 | 0.000 |
| 14 | 3 | 1 | 7.899 | 8.909 | 4.301 | 7.802 |
| 14 | 3 | 2 | 7.808 | 9.897 | -2.205 | -9.638 |

SYNLEUCITE

ALL REFLECTIONS

NUMERATOR

DENOMINATOR

NUMBER

WEIGHTED R

7002.06

2871307.50

978

UNWEIGHTED R

981.01

17163.88

978

RANGES OF F(OBS)

| | | |
|---------|------------|-----|
| 3304.79 | 2016961.38 | 687 |
| 1158.87 | 590115.38 | 201 |
| 700.05 | 182025.63 | 62 |
| 702.62 | 46974.36 | 16 |
| 3.62 | 5871.79 | 2 |
| 241.60 | 11743.59 | 4 |
| 719.91 | 14679.49 | 5 |
| 170.61 | 2935.90 | 1 |

RANGES OF (SIN(THETA)/LAMBDA)**2

| | | |
|---------|-----------|-----|
| 1811.69 | 184961.52 | 63 |
| 777.56 | 284782.03 | 97 |
| 484.06 | 381115.38 | 123 |
| 598.24 | 419833.28 | 143 |
| 637.94 | 393410.22 | 134 |
| 973.75 | 446256.34 | 152 |
| 773.97 | 396346.09 | 135 |
| 944.85 | 384602.56 | 131 |

UNREJECTED REFLECTIONS

WEIGHTED R

7002.06

2871307.50

978

UNWEIGHTED R

981.01

17163.88

978

RANGES OF F(OBS)

| | | |
|---------|------------|-----|
| 3304.79 | 2016961.38 | 687 |
| 1158.87 | 590115.38 | 201 |
| 700.05 | 182025.63 | 62 |
| 702.62 | 46974.36 | 16 |
| 3.62 | 5871.79 | 2 |
| 241.60 | 11743.59 | 4 |
| 719.91 | 14679.49 | 5 |
| 170.61 | 2935.90 | 1 |

RANGES OF (SIN(THETA)/LAMBDA)**2

| | | |
|---------|-----------|-----|
| 1811.69 | 184961.52 | 63 |
| 777.56 | 284782.03 | 97 |
| 484.06 | 381115.38 | 123 |
| 598.24 | 419833.28 | 143 |
| 637.94 | 393410.22 | 134 |
| 973.75 | 446256.34 | 152 |
| 773.97 | 396346.09 | 135 |
| 944.85 | 384602.56 | 131 |

SUM FCAL

17303.71

STANDARD DEV OF UNIT WEIGHT OBS

2.75