Neutron-diffraction study of bertrandite

Downs, and Ross

To be deposited: Table 8

American Mineralogist, 72, 9-10, 979-983
Table 8. Observed and calculated structure-factor moduli (calculated values on relative scale)

| H | K | L | $|F_o|^2$ | $|F_c|^2$ |
|---|---|---|---------|---------|
| -9 | -3 | 1 | 4226    | 4206    |
| -9 | 1  | 0 | 429     | 372     |
| -9 | 3  | 0 | 112     | 6       |
| -9 | 3  | 1 | 4193    | 4327    |
| -9 | 5  | 0 | 316     | 313     |
| -8 | -6 | 1 | 3872    | 3878    |
| -8 | -6 | 2 | 884     | 883     |
| -8 | -4 | 2 | 188     | 265     |
| -8 | 0  | 2 | 601     | 656     |
| -8 | 2  | 1 | 134     | 153     |
| -8 | 2  | 2 | 87      | 51      |
| -8 | 4  | 0 | 133     | 167     |
| -8 | 4  | 2 | 252     | 266     |
| -8 | 6  | 0 | 218     | 222     |
| -8 | 6  | 1 | 3948    | 4284    |
| -8 | 6  | 2 | 975     | 949     |
| -8 | 8  | 0 | 199     | 196     |
| -8 | 8  | 1 | 106     | 120     |
| -7 | -9 | 1 | 430     | 430     |
| -7 | -9 | 2 | 4559    | 4776    |
| -7 | -3 | 1 | 11103   | 10981   |
| -7 | -3 | 2 | 2731    | 3095    |
| -7 | -3 | 3 | 3862    | 4009    |
| -7 | -1 | 2 | 114     | 164     |
| -7 | 1  | 2 | 137     | 164     |
| -7 | 3  | 0 | 1760    | 1611    |
| -7 | 3  | 1 | 10757   | 12381   |
| -7 | 3  | 2 | 3055    | 3212    |
| -7 | 3  | 3 | 4100    | 4171    |
| -7 | 9  | 0 | 1951    | 2079    |
| -7 | 9  | 1 | 383     | 431     |
| -7 | 9  | 2 | 4636    | 5027    |
| -6 | -12| 1 | 4467    | 4226    |
| -6 | -8 | 2 | 126     | 113     |
| -6 | -6 | 1 | 7864    | 7560    |
| -6 | -6 | 2 | 5673    | 5588    |
| -6 | -6 | 3 | 5451    | 5696    |
| -6 | -4 | 2 | 175     | 178     |
| -6 | -2 | 1 | 232     | 293     |
| -6 | -2 | 3 | 536     | 555     |
| -6 | 0  | 2 | 17996   | 17996   |
| -6 | 0  | 4 | 9893    | 9621    |
| -6 | 2  | 1 | 234     | 294     |
| -6 | 2  | 3 | 524     | 557     |
| -6 | 4  | 0 | 794     | 716     |
| -6 | 4  | 1 | 55      | 89      |
| -6 | 4  | 2 | 142     | 179     |
| -6 | 6  | 0 | 9093    | 9712    |
| -6 | 6  | 1 | 8087    | 9306    |
| -6 | 6  | 2 | 6542    | 6426    |
| -6 | 6  | 3 | 5902    | 5984    |
| -6 | 8  | 0 | 167     | 210     |
| -6 | 10 | 1 | 185     | 183     |
| -6 | 12 | 1 | 3766    | 4262    |
| -6 | 12 | 2 | 3312    | 3410    |
| -5 | -13| 2 | 307     | 346     |
| -5 | -11| 3 | 167     | 222     |
| -5 | -9 | 1 | 11149   | 11485   |
| -5 | -9 | 2 | 5190    | 5366    |
| -5 | -9 | 3 | 5130    | 5638    |
| H | K | L | $|F_0|^2$ | $|F_0|^2$ |
|---|---|---|--------|--------|
| -5 | -7 | 2 | 69 | 5 |
| -5 | -5 | 4 | 188 | 192 |
| -5 | -3 | 1 | 5747 | 5520 |
| -5 | -3 | 2 | 4004 | 4261 |
| -5 | -5 | 3 | 17683 | 16070 |
| -5 | -3 | 4 | 2081 | 2234 |
| -5 | -1 | 2 | 359 | 412 |
| -5 | 1 | 1 | 83 | 80 |
| -5 | 1 | 2 | 364 | 412 |
| -5 | 3 | 0 | 12949 | 13154 |
| -5 | 3 | 1 | 6375 | 6655 |
| -5 | 3 | 2 | 4650 | 4381 |
| -5 | 3 | 3 | 18373 | 17406 |
| -5 | 3 | 4 | 2322 | 2249 |
| -5 | 5 | 0 | 235 | 247 |
| -5 | 5 | 4 | 198 | 192 |
| -5 | 7 | 1 | 141 | 184 |
| -5 | 7 | 3 | 152 | 136 |
| -5 | 9 | 0 | 16568 | 19391 |
| -5 | 9 | 1 | 10073 | 11958 |
| -5 | 9 | 2 | 5151 | 5458 |
| -5 | 9 | 3 | 5741 | 5677 |
| -5 | 11 | 2 | 74 | 57 |
| -5 | 11 | 3 | 230 | 222 |
| -5 | 13 | 1 | 133 | 90 |
| -5 | 13 | 2 | 328 | 346 |
| -4 | -12 | 1 | 2094 | 2046 |
| -4 | -12 | 2 | 4237 | 3967 |
| -4 | -12 | 3 | 573 | 623 |
| -4 | -10 | 1 | 153 | 176 |
| -4 | -10 | 2 | 211 | 288 |
| -4 | -8 | 3 | 137 | 155 |
| -4 | -6 | 1 | 4793 | 5049 |
| -4 | -6 | 2 | 1713 | 1813 |
| -4 | -6 | 3 | 815 | 796 |
| -4 | -6 | 4 | 1647 | 1616 |
| -4 | -4 | 2 | 102 | 192 |
| -4 | -4 | 4 | 130 | 115 |
| -4 | 0 | 2 | 4867 | 5140 |
| -4 | 0 | 4 | 6163 | 6190 |
| -4 | 2 | 0 | 110 | 143 |
| -4 | 4 | 2 | 199 | 193 |
| -4 | 4 | 4 | 177 | 115 |
| -4 | 6 | 0 | 1582 | 1807 |
| -4 | 6 | 1 | 4588 | 5292 |
| -4 | 6 | 2 | 1838 | 1829 |
| -4 | 6 | 3 | 771 | 797 |
| -4 | 6 | 4 | 1613 | 1619 |
| -4 | 8 | 3 | 162 | 155 |
| -4 | 10 | 0 | 93 | 29 |
| -4 | 10 | 2 | 245 | 288 |
| -4 | 12 | 0 | 966 | 1219 |
| -4 | 12 | 1 | 1748 | 2048 |
| -4 | 12 | 1 | 3504 | 3964 |
| -4 | 12 | 3 | 601 | 623 |
| -4 | 14 | 0 | 264 | 349 |
| -3 | -15 | 1 | 14015 | 12814 |
| -3 | -15 | 2 | 2691 | 2562 |
| -3 | -13 | 1 | 187 | 196 |
| -3 | -13 | 2 | 371 | 467 |
| H  | K  | L  | |Fo|^2 | |Fe|^2 |
|----|----|----|-----|-----|-----|
| -3 | -11 | 1  | 554 | 547 |
| -3 | -11 | 3  | 144 | 236 |
| -3 | -9  | 1  | 1888| 1702|
| -3 | -9  | 2  | 13883| 13502|
| -3 | -9 | 3  | 4739 | 4802 |
| -3 | -9 | 4  | 3965 | 3924 |
| -3 | -7 | 1  | 540 | 665 |
| -3 | -7 | 2  | 162 | 119 |
| -3 | -7 | 3  | 794 | 873 |
| -3 | -5 | 2  | 480 | 524 |
| -3 | -5 | 4  | 189 | 142 |
| -3 | -3 | 1  | 2603 | 2823 |
| -3 | -3 | 2  | 4724 | 5186 |
| -3 | -3 | 3  | 14391 | 14460 |
| -3 | -3 | 4  | 542 | 574 |
| -3 | -1 | 1  | 185 | 237 |
| -3 | -1 | 2  | 93 | 110 |
| -3 | -1 | 3  | 246 | 296 |
| -3 | -1 | 4  | 215 | 231 |
| -3 | 0  | 810 | 821 |
| -3 | 1  | 1  | 221 | 237 |
| -3 | 1  | 2  | 149 | 111 |
| -3 | 1  | 3  | 323 | 296 |
| -3 | 1  | 4  | 187 | 231 |
| -3 | 2  | 9601 | 9666 |
| -3 | 3  | 3220 | 3185 |
| -3 | 3  | 5572 | 5250 |
| -3 | 3  | 15161 | 14709 |
| -3 | 3  | 4  | 542 | 574 |
| -3 | 5  | 276 | 365 |
| -3 | 5  | 492 | 524 |
| -3 | 5  | 88 | 111 |
| -3 | 5  | 140 | 142 |
| -3 | 7  | 1  | 590 | 666 |
| -3 | 7  | 3  | 874 | 873 |
| -3 | 9  | 23641 | 25842 |
| -3 | 9  | 1  | 1664 | 1704 |
| -3 | 9  | 12790 | 13475 |
| -3 | 9  | 4700 | 4779 |
| -3 | 9  | 3923 | 3915 |
| -3 | 11 | 486 | 546 |
| -3 | 11 | 3  | 255 | 235 |
| -3 | 13 | 0  | 1138 | 1180 |
| -3 | 13 | 1  | 129 | 196 |
| -3 | 13 | 2  | 473 | 467 |
| -3 | 15 | 0  | 160 | 137 |
| -3 | 15 | 1  | 11347 | 12759 |
| -2 | 15 | 2  | 2129 | 2557 |
| -2 | 16 | 1  | 221 | 184 |
| -2 | -12 | 1  | 3959 | 3752 |
| -2 | -12 | 2  | 15719 | 14570 |
| -2 | -12 | 3  | 2720 | 2542 |
| -2 | -10 | 1  | 384 | 395 |
| -2 | -10 | 2  | 362 | 416 |
| -2 | -8 | 1  | 116 | 120 |
| -2 | -8 | 2  | 169 | 176 |
| -2 | -8 | 3  | 232 | 306 |
| -2 | -6 | 1  | 8758 | 8449 |
| -2 | -6 | 2  | 1446 | 1439 |
| -2 | -6 | 3  | 19696 | 20012 |
| H  | K  | L  | $|F_o|^2$ | $|F_e|^2$ |
|----|----|----|---------|---------|
| -2 | -6 | 4  | 1879    | 2090    |
| -2 | -4 | 2  | 449     | 492     |
| -2 | -4 | 4  | 243     | 259     |
| 0  | -20| 1  | 476     | 455     |
| 0  | -18| 1  | 5325    | 4921    |
| 0  | -18| 2  | 4829    | 4864    |
| 0  | -16| 1  | 401     | 349     |
| 0  | -16| 2  | 277     | 242     |
| 0  | -16| 3  | 326     | 337     |
| 0  | -16| 4  | 162     | 202     |
| 0  | -14| 1  | 168     | 193     |
| 0  | -14| 2  | 243     | 242     |
| 0  | -14| 4  | 255     | 162     |
| 0  | -12| 1  | 5868    | 5488    |
| 0  | -12| 2  | 4526    | 4319    |
| 0  | -12| 3  | 8363    | 8375    |
| 0  | -12| 4  | 7302    | 7592    |
| 0  | -10| 1  | 200     | 186     |
| 0  | -10| 3  | 306     | 342     |
| 0  | -10| 5  | 166     | 153     |
| 0  | -8 | 1  | 178     | 185     |
| 0  | -8 | 2  | 241     | 240     |
| 0  | -8 | 4  | 214     | 221     |
| 0  | -6 | 1  | 7704    | 7294    |
| 0  | -6 | 2  | 8681    | 8311    |
| 0  | -6 | 3  | 28008   | 28862   |
| 0  | -6 | 4  | 3093    | 3156    |
| 0  | -6 | 5  | 15474   | 15461   |
| 0  | -4 | 2  | 263     | 318     |
| 0  | -4 | 3  | 141     | 146     |
| 0  | -4 | 4  | 209     | 248     |
| 0  | -4 | 5  | 132     | 88      |
| 0  | -2 | 1  | 455     | 416     |
| 0  | -2 | 3  | 557     | 622     |
| 0  | -2 | 4  | 62      | 67      |
| 0  | -2 | 5  | 446     | 460     |
| 0  | 0  | 2   | 24432   | 22648   |
| 0  | 0  | 4   | 772     | 773     |
| 0  | 0  | 6   | 17106   | 17367   |
| 0  | 2  | 1   | 450     | 415     |
| 0  | 2  | 2   | 120     | 89      |
| 0  | 2  | 3   | 602     | 621     |
| 0  | 2  | 5   | 445     | 460     |
| 0  | 4  | 0   | 858     | 835     |
| 0  | 4  | 1   | 160     | 136     |
| 0  | 4  | 2   | 330     | 317     |
| 0  | 4  | 3   | 119     | 146     |
| 0  | 4  | 4   | 241     | 248     |
| 0  | 4  | 5   | 104     | 88      |
| 0  | 4  | 6   | 195     | 176     |
| 0  | 6  | 0   | 12423   | 12160   |
| 0  | 6  | 1   | 7590    | 7208    |
| 0  | 6  | 2   | 8675    | 8186    |
| 0  | 6  | 3   | 29081   | 27752   |
| 0  | 6  | 4   | 3172    | 3143    |
| 0  | 6  | 5   | 14977   | 15269   |
| 0  | 6  | 6   | 1050    | 913     |
| 0  | 8  | 0   | 230     | 246     |
| 0  | 8  | 1   | 191     | 185     |
| 0  | 8  | 2   | 212     | 240     |
|   |   |   | $|F_o|^{2}$ | $|F_c|^{2}$ |
|---|---|---|----------|----------|
| 0 | 8 | 3 | 125      | 61       |
| 0 | 8 | 4 | 234      | 220      |
| 0 | 8 | 5 | 174      | 168      |
| 0 | 10| 0 | 321      | 296      |
| 0 | 10| 1 | 197      | 186      |
| 0 | 10| 2 | 50       | 76       |
| 0 | 10| 3 | 364      | 342      |
| 0 | 10| 4 | 231      | 259      |
| 0 | 10| 5 | 146      | 153      |
| 0 | 12| 0 | 15229    | 14453    |
| 0 | 12| 1 | 5795     | 5471     |
| 0 | 12| 2 | 4514     | 4299     |
| 0 | 12| 3 | 8547     | 8284     |
| 0 | 12| 4 | 7545     | 7515     |
| 0 | 12| 5 | 4337     | 4541     |
| 0 | 14| 1 | 177      | 193      |
| 0 | 14| 2 | 214      | 242      |
| 0 | 14| 3 | 72       | 50       |
| 0 | 14| 4 | 188      | 162      |
| 0 | 16| 0 | 517      | 493      |
| 0 | 16| 1 | 331      | 349      |
| 0 | 16| 2 | 224      | 242      |
| 0 | 16| 3 | 364      | 337      |
| 0 | 16| 4 | 273      | 202      |
| 0 | 18| 0 | 7778     | 7644     |
| 0 | 18| 1 | 5289     | 4916     |
| 0 | 18| 2 | 4868     | 4850     |
| 0 | 18| 3 | 13836    | 14298    |
| 0 | 20| 0 | 67       | 42       |
| 1 | -19| 1 | 401      | 405      |
| 1 | -17| 2 | 81       | 131      |
| 1 | -15| 1 | 1358     | 1243     |
| 1 | -15| 2 | 1405     | 1319     |
| 1 | -15| 3 | 3741     | 3770     |
| 1 | -15| 4 | 319      | 353      |
| 1 | -13| 1 | 81       | 81       |
| 1 | -13| 2 | 254      | 272      |
| 1 | -13| 3 | 63       | 75       |
| 1 | -11| 3 | 153      | 170      |
| 1 | -9 | 1 | 6050     | 5647     |
| 1 | -9 | 2 | 1739     | 1536     |
| 1 | -9 | 3 | 1624     | 1743     |
| 1 | -9 | 4 | 1745     | 1763     |
| 1 | -9 | 5 | 504      | 495      |
| 1 | -7 | 1 | 235      | 193      |
| 1 | -7 | 3 | 59       | 106      |
| 1 | -7 | 5 | 202      | 293      |
| 1 | -5 | 1 | 108      | 78       |
| 1 | -5 | 4 | 180      | 151      |
| 1 | -3 | 1 | 6957     | 6719     |
| 1 | -3 | 3 | 9506     | 9645     |
| 1 | -3 | 4 | 815      | 829      |
| 1 | -3 | 5 | 3065     | 2994     |
| 1 | -3 | 6 | 1476     | 1332     |
| 1 | -1| 2 | 392      | 419      |
| 1 | 1 | 2 | 411      | 419      |
| 1 | 1 | 4 | 116      | 78       |
| 1 | 3 | 0 | 4064     | 4333     |
| 1 | 3 | 1 | 6849     | 6671     |
| H  | K  | L  | $|F_o|^2$ | $|F_c|^2$ |
|----|----|----|--------|--------|
| 1  | 3  | 2  | 822    | 763    |
| 1  | 3  | 3  | 9745   | 9525   |
| 1  | 3  | 4  | 836    | 829    |
| 1  | 3  | 5  | 2989   | 2990   |
| 1  | 3  | 6  | 1306   | 1331   |
| 1  | 5  | 0  | 204    | 187    |
| 1  | 5  | 3  | 98     | 107    |
| 1  | 5  | 4  | 164    | 151    |
| 1  | 5  | 5  | 155    | 142    |
| 1  | 7  | 1  | 212    | 193    |
| 1  | 7  | 3  | 179    | 106    |
| 1  | 7  | 5  | 192    | 203    |
| 1  | 9  | 0  | 6008   | 5872   |
| 1  | 9  | 1  | 6035   | 5621   |
| 1  | 9  | 2  | 1596   | 1533   |
| 1  | 9  | 3  | 1894   | 1739   |
| 1  | 9  | 4  | 1795   | 1758   |
| 1  | 9  | 5  | 547    | 494    |
| 1  | 11 | 1  | 103    | 92     |
| 1  | 11 | 2  | 144    | 72     |
| 1  | 11 | 3  | 169    | 170    |
| 1  | 13 | 2  | 286    | 272    |
| 1  | 13 | 3  | 149    | 75     |
| 1  | 15 | 0  | 822    | 806    |
| 1  | 15 | 1  | 1322   | 1242   |
| 1  | 15 | 2  | 1358   | 1318   |
| 1  | 15 | 3  | 3877   | 3756   |
| 1  | 15 | 4  | 371    | 353    |
| 1  | 17 | 0  | 454    | 424    |
| 1  | 17 | 1  | 9      | 45     |
| 1  | 17 | 2  | 172    | 131    |
| 1  | 19 | 0  | 101    | 39     |
| 1  | 19 | 1  | 411    | 405    |
| 2  | -18| 1  | 7666   | 8120   |
| 2  | -18| 2  | 8211   | 8405   |
| 2  | -16| 1  | 293    | 184    |
| 2  | -16| 2  | 149    | 113    |
| 2  | -16| 3  | 225    | 216    |
| 2  | -14| 2  | 95     | 102    |
| 2  | -12| 1  | 3694   | 3761   |
| 2  | -12| 2  | 14845  | 14741  |
| 2  | -12| 3  | 2609   | 2548   |
| 2  | -12| 4  | 620    | 599    |
| 2  | -10| 1  | 372    | 395    |
| 2  | -10| 2  | 432    | 417    |
| 2  | -10| 3  | 62     | 8      |
| 2  | -10| 5  | 270    | 227    |
| 2  | -8 | 3  | 313    | 306    |
| 2  | -6 | 1  | 8831   | 8690   |
| 2  | -6 | 2  | 1474   | 1447   |
| 2  | -6 | 3  | 20207  | 21118  |
| 2  | -6 | 4  | 1993   | 2103   |
| 2  | -6 | 5  | 7573   | 7478   |
| 2  | -4 | 2  | 572    | 494    |
| 2  | -4 | 3  | 134    | 142    |
| 2  | -4 | 4  | 226    | 259    |
| 2  | -4 | 5  | 76     | 85     |
| 2  | -2 | 1  | 267    | 242    |
| 2  | -2 | 4  | 161    | 136    |
| 2  | -2 | 5  | 129    | 147    |
| H | K | L | $|Fo|^2$ | $|Fc|^2$ |
|---|---|---|--------|--------|
| 2 | 0 | 0 | 12380  | 11901  |
| 2 | 0 | 2 | 4174   | 4063   |
| 2 | 0 | 4 | 10763  | 10885  |
| 2 | 0 | 6 | 18139  | 18685  |
| 2 | 2 | 0 | 122    | 135    |
| 2 | 2 | 1 | 272    | 242    |
| 2 | 2 | 2 | 105    | 61     |
| 2 | 2 | 3 | 121    | 36     |
| 2 | 2 | 4 | 109    | 137    |
| 2 | 2 | 5 | 151    | 147    |
| 2 | 2 | 6 | 144    | 154    |
| 2 | 4 | 1 | 99     | 58     |
| 2 | 4 | 2 | 511    | 494    |
| 2 | 4 | 3 | 121    | 142    |
| 2 | 4 | 4 | 251    | 259    |
| 2 | 4 | 5 | 118    | 85     |
| 2 | 6 | 0 | 937    | 786    |
| 2 | 6 | 1 | 9113   | 8621   |
| 2 | 6 | 2 | 1572   | 1445   |
| 2 | 6 | 3 | 20878  | 20817  |
| 2 | 6 | 4 | 2066   | 2098   |
| 2 | 6 | 5 | 7244   | 7427   |
| 2 | 8 | 0 | 116    | 134    |
| 2 | 8 | 1 | 123    | 120    |
| 2 | 8 | 2 | 147    | 176    |
| 2 | 8 | 3 | 288    | 306    |
| 2 | 8 | 4 | 36     | 37     |
| 2 | 10| 0 | 132    | 129    |
| 2 | 10| 1 | 387    | 395    |
| 2 | 10| 2 | 453    | 416    |
| 2 | 10| 5 | 210    | 227    |
| 2 | 12| 0 | 33310  | 32356  |
| 2 | 12| 1 | 3958   | 3754   |
| 2 | 12| 2 | 15465  | 14585  |
| 2 | 12| 3 | 2761   | 2542   |
| 2 | 12| 4 | 601    | 598    |
| 2 | 12| 5 | 2304   | 2279   |
| 2 | 14| 0 | 531    | 507    |
| 2 | 14| 2 | 104    | 102    |
| 2 | 14| 3 | 144    | 94     |
| 2 | 16| 0 | 132    | 182    |
| 2 | 16| 1 | 104    | 184    |
| 2 | 16| 2 | 171    | 113    |
| 2 | 16| 3 | 228    | 216    |
| 2 | 18| 0 | 10205  | 9655   |
| 2 | 18| 1 | 8073   | 8112   |
| 2 | 18| 2 | 8609   | 8373   |
| 2 | 18| 3 | 7433   | 8105   |
| 3 | -19| 2 | 337    | 333    |
| 3 | -17| 1 | 175    | 190    |
| 3 | -15| 1 | 12295  | 12885  |
| 3 | -15| 2 | 2520   | 2567   |
| 3 | -15| 3 | 22503  | 24103  |
| 3 | -13| 1 | 171    | 196    |
| 3 | -13| 2 | 475    | 467    |
| 3 | -13| 4 | 531    | 504    |
| 3 | -11| 1 | 592    | 547    |
| 3 | -11| 3 | 277    | 236    |
| 2 | -9 | 1 | 1778   | 1708   |
| 3 | -9 | 2 | 13424  | 13966  |
| H | K | L | $|\text{Fo}|^2$ | $|\text{Fe}|^2$ |
|---|---|---|-------|-------|
| 3 | -9 | 3 | 4838  | 4865  |
| 3 | -9 | 4 | 4006  | 3978  |
| 3 | -9 | 5 | 5538  | 5380  |
| 3 | -7 | 1 | 710   | 667   |
| 3 | -7 | 3 | 1001  | 876   |
| 3 | -7 | 5 | 336   | 324   |
| 3 | -5 | 2 | 581   | 526   |
| 3 | -5 | 3 | 115   | 111   |
| 3 | -5 | 4 | 142   | 142   |
| 3 | -3 | 1 | 3461  | 3278  |
| 3 | -3 | 2 | 5660  | 5601  |
| 3 | -3 | 3 | 15604 | 16402 |
| 3 | -3 | 4 | 597   | 576   |
| 3 | -3 | 5 | 9698  | 9569  |
| 3 | -1 | 1 | 196   | 238   |
| 3 | -1 | 2 | 114   | 111   |
| 3 | -1 | 3 | 340   | 297   |
| 3 | -1 | 4 | 337   | 231   |
| 3 | -1 | 5 | 257   | 272   |
| 3 | 1  | 0 | 639   | 813   |
| 3 | 1  | 1 | 228   | 238   |
| 3 | 1  | 2 | 106   | 111   |
| 3 | 1  | 3 | 323   | 297   |
| 3 | 1  | 4 | 234   | 231   |
| 3 | 1  | 5 | 277   | 272   |
| 3 | 3  | 0 | 8570  | 8805  |
| 3 | 3  | 1 | 3405  | 3298  |
| 3 | 3  | 2 | 5878  | 5616  |
| 3 | 3  | 3 | 15946 | 16152 |
| 3 | 3  | 4 | 604   | 576   |
| 3 | 3  | 5 | 9399  | 9528  |
| 3 | 3  | 6 | 7036  | 6487  |
| 3 | 5  | 0 | 355   | 364   |
| 3 | 5  | 1 | 156   | 112   |
| 3 | 5  | 2 | 547   | 526   |
| 3 | 5  | 3 | 144   | 111   |
| 3 | 5  | 4 | 156   | 142   |
| 3 | 7  | 0 | 103   | 112   |
| 3 | 7  | 1 | 672   | 667   |
| 3 | 7  | 2 | 107   | 119   |
| 3 | 7  | 3 | 948   | 876   |
| 3 | 7  | 5 | 347   | 324   |
| 3 | 9  | 0 | 27517 | 25356 |
| 3 | 9  | 1 | 2017  | 1706  |
| 3 | 9  | 2 | 14635 | 13866 |
| 3 | 9  | 3 | 5040  | 4851  |
| 3 | 9  | 4 | 3955  | 3957  |
| 3 | 9  | 5 | 5190  | 5349  |
| 3 | 11 | 1 | 555   | 547   |
| 3 | 11 | 3 | 247   | 236   |
| 3 | 11 | 4 | 141   | 66    |
| 3 | 11 | 5 | 157   | 172   |
| 3 | 13 | 0 | 1048  | 1179  |
| 3 | 13 | 1 | 190   | 196   |
| 3 | 13 | 2 | 468   | 467   |
| 3 | 13 | 3 | 84    | 22    |
| 3 | 13 | 4 | 497   | 504   |
| 3 | 15 | 0 | 174   | 137   |
| 3 | 15 | 1 | 13472 | 12845 |
| 3 | 15 | 2 | 2693  | 2564  |
| H | K | L | \(|Fo|^2\) | \(|Fe|^2\) |
|---|---|---|---------|---------|
| 3 | 15 | 3 | 22587   | 23816   |
| 3 | 15 | 4 | 4196    | 4551    |
| 3 | 17 | 1 | 195     | 190     |
| 3 | 17 | 2 | 197     | 134     |
| 3 | 17 | 3 | 152     | 131     |
| 3 | 19 | 0 | 292     | 213     |
| 3 | 19 | 2 | 93      | 98      |
| 3 | 19 | 2 | 360     | 333     |
| 3 | -18| 1 | 1557    | 1546    |
| 4 | -16| 1 | 208     | 205     |
| 4 | -16| 3 | 26      | 80      |
| 4 | -14| 2 | 134     | 106     |
| 4 | -14| 3 | 100     | 66      |
| 4 | -12| 1 | 2104    | 2052    |
| 4 | -12| 2 | 4070    | 3998    |
| 4 | -12| 3 | 695     | 624     |
| 4 | -12| 4 | 7353    | 7305    |
| 4 | -10| 1 | 136     | 176     |
| 4 | -10| 2 | 314     | 288     |
| 4 | -8 | 3 | 166     | 155     |
| 4 | -6 | 1 | 5354    | 5350    |
| 4 | -6 | 2 | 1947    | 1848    |
| 4 | -6 | 3 | 806     | 801     |
| 4 | -6 | 4 | 1685    | 1633    |
| 4 | -6 | 5 | 2447    | 2311    |
| 4 | -4 | 1 | 132     | 112     |
| 4 | -4 | 2 | 209     | 193     |
| 4 | -4 | 4 | 76      | 115     |
| 4 | -2 | 1 | 153     | 124     |
| 4 | 2  | 2 | 94      | 90      |
| 4 | 0  | 0 | 1829    | 2028    |
| 4 | 0  | 2 | 5972    | 5602    |
| 4 | 0  | 4 | 6652    | 6468    |
| 4 | 2  | 0 | 130     | 142     |
| 4 | 2  | 1 | 155     | 124     |
| 4 | 4  | 1 | 103     | 112     |
| 4 | 4  | 2 | 206     | 193     |
| 4 | 4  | 3 | 51      | 64      |
| 4 | 4  | 4 | 136     | 115     |
| 4 | 4  | 5 | 56      | 36      |
| 4 | 6  | 0 | 1738    | 1791    |
| 4 | 6  | 1 | 5423    | 5340    |
| 4 | 6  | 2 | 2040    | 1849    |
| 4 | 6  | 3 | 818     | 801     |
| 4 | 6  | 4 | 1616    | 1630    |
| 4 | 6  | 5 | 2393    | 2307    |
| 4 | 8  | 0 | 133     | 119     |
| 4 | 8  | 1 | 151     | 66      |
| 4 | 8  | 2 | 100     | 66      |
| 4 | 8  | 3 | 132     | 155     |
| 4 | 10 | 1 | 166     | 176     |
| 4 | 10 | 2 | 289     | 288     |
| 4 | 12 | 0 | 1302    | 1218    |
| 4 | 12 | 1 | 2113    | 2050    |
| 4 | 12 | 2 | 4217    | 3993    |
| 4 | 12 | 3 | 580     | 624     |
| 4 | 12 | 4 | 6913    | 7252    |
| 4 | 14 | 0 | 324     | 349     |
| 4 | 14 | 3 | 111     | 66      |
| 4 | 16 | 0 | 135     | 73      |
| H | K | L | |Fo|² | |Fc|² |
|---|---|---|---|---|---|---|
| 4 | 16 | 1 | 184 | 205 |
| 4 | 18 | 0 | 3422 | 3936 |
| 4 | 18 | 1 | 1452 | 1545 |
| 4 | 18 | 2 | 4380 | 4463 |
| 5 | -13 | 1 | 50 | 96 |
| 5 | -13 | 2 | 323 | 346 |
| 5 | -11 | 3 | 242 | 222 |
| 5 | -9 | 1 | 11217 | 12112 |
| 5 | -9 | 2 | 5372 | 5550 |
| 5 | -9 | 3 | 5917 | 5832 |
| 5 | -8 | 2 | 5917 | 5832 |
| 5 | -7 | 1 | 182 | 184 |
| 5 | -7 | 3 | 111 | 136 |
| 5 | -5 | 4 | 210 | 192 |
| 5 | -3 | 1 | 6775 | 7031 |
| 5 | -3 | 2 | 4776 | 4823 |
| 5 | -3 | 3 | 18130 | 20201 |
| 5 | -3 | 4 | 2401 | 2284 |
| 5 | -1 | 2 | 412 | 414 |
| 5 | -1 | 4 | 102 | 85 |
| 5 | 1 | 1 | 101 | 80 |
| 5 | 1 | 2 | 379 | 415 |
| 5 | 1 | 3 | 109 | 84 |
| 5 | 1 | 4 | 278 | 85 |
| 5 | 3 | 0 | 12312 | 12405 |
| 5 | 3 | 1 | 7103 | 7085 |
| 5 | 3 | 2 | 5061 | 4838 |
| 5 | 3 | 3 | 19383 | 20022 |
| 5 | 3 | 4 | 2318 | 2281 |
| 5 | 3 | 5 | 8325 | 8907 |
| 5 | 5 | 0 | 214 | 247 |
| 5 | 5 | 2 | 129 | 34 |
| 5 | 5 | 3 | 137 | 135 |
| 5 | 5 | 4 | 187 | 192 |
| 5 | 5 | 5 | 159 | 194 |
| 5 | 7 | 1 | 189 | 184 |
| 5 | 7 | 3 | 164 | 136 |
| 5 | 9 | 0 | 18703 | 18669 |
| 5 | 9 | 1 | 12157 | 12020 |
| 5 | 9 | 2 | 5352 | 5551 |
| 5 | 9 | 3 | 5885 | 5831 |
| 5 | 9 | 4 | 2260 | 2378 |
| 5 | 11 | 1 | 163 | 99 |
| 5 | 11 | 2 | 81 | 57 |
| 5 | 11 | 3 | 204 | 222 |
| 5 | 13 | 1 | 121 | 91 |
| 5 | 13 | 2 | 300 | 346 |
| 5 | 15 | 0 | 4104 | 3805 |
| 5 | 15 | 1 | 5916 | 5509 |
| 5 | 15 | 2 | 5971 | 5711 |
| 5 | 15 | 3 | 13248 | 13666 |
| 5 | 17 | 0 | 438 | 467 |
| 5 | 17 | 2 | 244 | 156 |
| 6 | -12 | 1 | 4176 | 4274 |
| 6 | -12 | 2 | 3605 | 3436 |
| 6 | -10 | 2 | 145 | 94 |
| 6 | -8 | 2 | 129 | 113 |
| 6 | -8 | 3 | 164 | 95 |
| 6 | -6 | 1 | 8979 | 9360 |
| 6 | -6 | 2 | 6656 | 6684 |
| H | K | L | $|Fo|^2$ | $|Fc|^2$ |
|---|---|---|--------|--------|
| 6  | -6 | 3 | 6297   | 6253   |
| 6  | -4 | 1 | 134    | 89     |
| 6  | -4 | 2 | 174    | 179    |
| 6  | -2 | 1 | 308    | 294    |
| 6  | -2 | 2 | 65     | 76     |
| 6  | -2 | 3 | 594    | 560    |
| 6  | 0  | 0 | 16490  | 16532  |
| 6  | 0  | 2 | 20443  | 21348  |
| 6  | 0  | 4 | 10783  | 10514  |
| 6  | 2  | 1 | 210    | 294    |
| 6  | 2  | 2 | 123    | 76     |
| 6  | 2  | 3 | 568    | 560    |
| 6  | 2  | 4 | 86     | 72     |
| 6  | 4  | 0 | 694    | 714    |
| 6  | 4  | 1 | 117    | 89     |
| 6  | 4  | 2 | 185    | 179    |
| 6  | 4  | 3 | 66     | 55     |
| 6  | 6  | 0 | 8927   | 9203   |
| 6  | 6  | 1 | 9328   | 9345   |
| 6  | 6  | 2 | 6759   | 6717   |
| 6  | 6  | 3 | 6338   | 6245   |
| 6  | 8  | 0 | 202    | 210    |
| 6  | 8  | 2 | 132    | 113    |
| 6  | 8  | 3 | 117    | 96     |
| 6  | 10 | 0 | 81     | 104    |
| 6  | 10 | 1 | 147    | 163    |
| 6  | 10 | 2 | 130    | 94     |
| 6  | 12 | 0 | 176    | 145    |
| 6  | 12 | 1 | 3777   | 4265   |
| 6  | 12 | 2 | 3148   | 3427   |
| 6  | 16 | 0 | 574    | 567    |
| 6  | 16 | 1 | 346    | 330    |
| 7  | -15| 1 | 1973   | 1931   |
| 7  | -9 | 1 | 466    | 431    |
| 7  | -9 | 2 | 5242   | 5104   |
| 7  | -9 | 3 | 3911   | 3624   |
| 7  | -7 | 1 | 127    | 83     |
| 7  | -3 | 1 | 12492  | 12745  |
| 7  | -3 | 2 | 3515   | 3298   |
| 7  | -3 | 3 | 4434   | 4326   |
| 7  | -3 | 4 | 4555   | 3937   |
| 7  | -1 | 2 | 160    | 164    |
| 7  | 1  | 2 | 170    | 164    |
| 7  | 3  | 0 | 1544   | 1598   |
| 7  | 3  | 1 | 12535  | 12759  |
| 7  | 3  | 2 | 3418   | 3302   |
| 7  | 3  | 3 | 4456   | 4321   |
| 7  | 3  | 4 | 4018   | 3930   |
| 7  | 5  | 0 | 84     | 59     |
| 7  | 5  | 4 | 80     | 63     |
| 7  | 7  | 1 | 87     | 83     |
| 7  | 9  | 0 | 1952   | 2062   |
| 7  | 9  | 1 | 420    | 431    |
| 7  | 9  | 2 | 4985   | 5115   |
| 7  | 9  | 3 | 3570   | 3625   |
| 7  | 11 | 1 | 54     | 58     |
| 7  | 13 | 0 | 82     | 2      |
| 7  | 13 | 2 | 62     | 81     |
| 7  | 15 | 0 | 1616   | 1680   |
| 8  | -12| 1 | 3978   | 3940   |
| H | K | L | $|F_o|^2$ | $|F_c|^2$ |
|---|---|---|--------|--------|
| 8 | -12 | 2 | 7531  | 7569  |
| 8 | -10 | 2 | 380   | 329   |
| 8 | -8  | 1 | 122   | 120   |
| 8 | -8  | 2 | 129   | 96    |
| 8 | -8  | 3 | 374   | 313   |
| 8 | -6  | 1 | 4294  | 4304  |
| 8 | -6  | 2 | 990   | 956   |
| 8 | -6  | 3 | 12426 | 12077 |
| 8 | -4  | 2 | 314   | 267   |
| 8 | -2  | 1 | 178   | 153   |
| 8 | -2  | 3 | 141   | 110   |
| 8 | -2  | 4 | 58    | 82    |
| 8 | 0   | 0 | 7627  | 7922  |
| 8 | 0   | 2 | 725   | 659   |
| 8 | 0   | 4 | 6474  | 6133  |
| 8 | 2   | 0 | 169   | 196   |
| 8 | 2   | 1 | 123   | 153   |
| 8 | 2   | 2 | 86    | 51    |
| 8 | 2   | 3 | 117   | 110   |
| 8 | 4   | 0 | 174   | 167   |
| 8 | 4   | 1 | 77    | 92    |
| 8 | 4   | 2 | 324   | 267   |
| 8 | 4   | 3 | 150   | 87    |
| 8 | 4   | 4 | 151   | 143   |
| 8 | 6   | 0 | 225   | 222   |
| 8 | 6   | 1 | 4255  | 4301  |
| 8 | 6   | 2 | 999   | 956   |
| 8 | 6   | 3 | 11831 | 12068 |
| 8 | 8   | 0 | 185   | 196   |
| 8 | 8   | 1 | 128   | 120   |
| 8 | 8   | 2 | 203   | 96    |
| 8 | 8   | 3 | 292   | 313   |
| 8 | 10  | 1 | 175   | 181   |
| 8 | 10  | 2 | 317   | 329   |
| 8 | 12  | 0 | 16098 | 17427 |
| 8 | 12  | 1 | 4058  | 3929  |
| 8 | 12  | 2 | 6954  | 7579  |
| 8 | 14  | 0 | 486   | 515   |
| 9 | -11 | 1 | 200   | 232   |
| 9 | -9  | 1 | 9404  | 9233  |
| 9 | -9  | 2 | 12246 | 11836 |
| 9 | -7  | 1 | 500   | 428   |
| 9 | -7  | 2 | 107   | 92    |
| 9 | -7  | 3 | 642   | 521   |
| 9 | -5  | 1 | 53    | 73    |
| 9 | -5  | 2 | 321   | 299   |
| 9 | -3  | 1 | 5049  | 4373  |
| 9 | -3  | 2 | 7680  | 6789  |
| 9 | -3  | 3 | 1283  | 1093  |
| 9 | -1  | 1 | 93    | 94    |
| 9 | -1  | 3 | 251   | 255   |
| 9 | 0   | 1 | 324   | 372   |
| 9 | 1   | 1 | 185   | 94    |
| 9 | 1   | 3 | 272   | 255   |
| 9 | 3   | 0 | 121   | 6     |
| 9 | 3   | 1 | 4792  | 4366  |
| 9 | 3   | 2 | 6668  | 6807  |
| 9 | 3   | 3 | 1022  | 1093  |
| 9 | 5   | 0 | 300   | 312   |
| 9 | 5   | 1 | 98    | 73    |
| H | K | L | $|F_o|^2$ | $|F_c|^2$ |
|---|---|---|---------|---------|
| 9 | 5 | 2 | 250     | 299     |
| 9 | 7 | 0 | 151     | 124     |
| 9 | 7 | 1 | 484     | 428     |
| 9 | 7 | 3 | 558     | 521     |
| 9 | 9 | 0 | 2202    | 2223    |
| 9 | 9 | 1 | 8392    | 9150    |
| 9 | 9 | 2 | 11986   | 11881   |
| 9 | 11| 1 | 283     | 232     |
| 10| -6| 1 | 4601    | 4213    |
| 10| -6| 2 | 1846    | 1663    |
| 10| 0 | 0 | 8347    | 7797    |
| 10| 0 | 2 | 7743    | 7257    |
| 10| 2 | 1 | 115     | 78      |
| 10| 4 | 1 | 26      | 33      |
| 10| 6 | 0 | 2222    | 2106    |
| 10| 6 | 1 | 4350    | 4206    |
| 10| 6 | 2 | 1578    | 1663    |
| 10| -3| 1 | 12057   | 10645   |
| 11| 3 | 0 | 1074    | 988     |
| 11| 3 | 1 | 11125   | 10567   |
| 11| 5 | 0 | 280     | 264     |