

Table 1. Observed and calculated structure factors for ercittite

| h k l | | | 10Fo | 10Fc | 10s | h k l | | | 10Fo | 10Fc | 10s | h k l | | | 10Fo | 10Fc | 10s | h k l | | | 10Fo | 10Fc | 10s | | | | | | |
|-------|----|---|------|------|-----|-------|----|---|------|------|-----|-------|----|---|------|------|-----|-------|---|----|------|------|-----|---|---|----|------|------|-----|
| 2 | 0 | 0 | 548 | 444 | 11 | 3 | 9 | 2 | 276 | 298 | 31 | 2 | 6 | 5 | 481 | 478 | 9 | 5 | 3 | 8 | 181 | 153 | 35 | 0 | 6 | 11 | 288 | 325 | 25 |
| 4 | 0 | 0 | 3722 | 3810 | 21 | 0 | 10 | 2 | 663 | 635 | 36 | 4 | 6 | 5 | 157 | 100 | 42 | 0 | 4 | 8 | 1683 | 1704 | 6 | 2 | 6 | 11 | 166 | 136 | 29 |
| 6 | 0 | 0 | 377 | 370 | 23 | 1 | 1 | 3 | 158 | 106 | 8 | 1 | 7 | 5 | 349 | 315 | 17 | 2 | 4 | 8 | 1122 | 1161 | 7 | 4 | 6 | 11 | 191 | 142 | 39 |
| 0 | 2 | 0 | 663 | 722 | 7 | 3 | 1 | 3 | 204 | 148 | 13 | 3 | 7 | 5 | 237 | 186 | 27 | 4 | 4 | 8 | 1023 | 1006 | 6 | 1 | 7 | 11 | 302 | 264 | 30 |
| 2 | 2 | 0 | 2494 | 2438 | 8 | 5 | 1 | 3 | 65 | 48 | 64 | 5 | 7 | 5 | 263 | 281 | 32 | 6 | 4 | 8 | 507 | 521 | 15 | 3 | 7 | 11 | 155 | 169 | 68 |
| 4 | 2 | 0 | 602 | 608 | 9 | 7 | 1 | 3 | 85 | 97 | 85 | 0 | 8 | 5 | 0 | 81 | 1 | 1 | 5 | 8 | 384 | 390 | 7 | 0 | 8 | 11 | 170 | 154 | 134 |
| 6 | 2 | 0 | 1222 | 1244 | 8 | 0 | 2 | 3 | 338 | 352 | 5 | 2 | 8 | 5 | 89 | 1 | 89 | 3 | 5 | 8 | 470 | 481 | 10 | 2 | 8 | 11 | 0 | 7 | 1 |
| 0 | 4 | 0 | 297 | 368 | 19 | 2 | 2 | 3 | 720 | 618 | 3 | 4 | 8 | 5 | 0 | 8 | 1 | 5 | 5 | 8 | 253 | 225 | 29 | 1 | 9 | 11 | 89 | 54 | 88 |
| 2 | 4 | 0 | 667 | 662 | 7 | 4 | 2 | 3 | 206 | 19 | 17 | 1 | 9 | 5 | 188 | 198 | 49 | 0 | 6 | 8 | 678 | 668 | 10 | 0 | 0 | 12 | 3009 | 3041 | 12 |
| 4 | 4 | 0 | 881 | 856 | 7 | 6 | 2 | 3 | 163 | 146 | 36 | 3 | 9 | 5 | 0 | 4 | 1 | 2 | 6 | 8 | 752 | 773 | 6 | 2 | 0 | 12 | 969 | 977 | 6 |
| 6 | 4 | 0 | 596 | 615 | 13 | 1 | 3 | 3 | 1088 | 1077 | 6 | 0 | 10 | 5 | 133 | 81 | 132 | 4 | 6 | 8 | 604 | 579 | 10 | 4 | 0 | 12 | 1756 | 1818 | 12 |
| 0 | 6 | 0 | 377 | 395 | 22 | 3 | 3 | 3 | 746 | 707 | 4 | 0 | 0 | 6 | 866 | 903 | 5 | 1 | 7 | 8 | 785 | 813 | 9 | 6 | 0 | 12 | 329 | 318 | 26 |
| 2 | 6 | 0 | 1670 | 1676 | 17 | 5 | 3 | 3 | 478 | 480 | 9 | 2 | 0 | 6 | 494 | 380 | 9 | 3 | 7 | 8 | 864 | 895 | 9 | 1 | 1 | 12 | 762 | 766 | 4 |
| 4 | 6 | 0 | 257 | 243 | 28 | 7 | 3 | 3 | 215 | 249 | 42 | 4 | 0 | 6 | 915 | 915 | 7 | 0 | 8 | 8 | 304 | 291 | 46 | 3 | 1 | 12 | 737 | 725 | 6 |
| 6 | 6 | 0 | 904 | 919 | 17 | 0 | 4 | 3 | 830 | 849 | 10 | 6 | 0 | 6 | 605 | 589 | 11 | 2 | 8 | 8 | 597 | 612 | 14 | 5 | 1 | 12 | 333 | 335 | 15 |
| 0 | 8 | 0 | 1317 | 1332 | 14 | 2 | 4 | 3 | 179 | 140 | 19 | 1 | 1 | 6 | 338 | 327 | 6 | 4 | 8 | 8 | 413 | 363 | 23 | 0 | 2 | 12 | 558 | 579 | 5 |
| 2 | 8 | 0 | 560 | 557 | 14 | 4 | 4 | 3 | 492 | 483 | 7 | 3 | 1 | 6 | 111 | 108 | 28 | 1 | 9 | 8 | 321 | 317 | 32 | 2 | 2 | 12 | 1626 | 1605 | 5 |
| 4 | 8 | 0 | 946 | 916 | 13 | 6 | 4 | 3 | 164 | 89 | 50 | 5 | 1 | 6 | 208 | 180 | 22 | 1 | 1 | 9 | 228 | 237 | 8 | 4 | 2 | 12 | 463 | 468 | 13 |
| 0 | 10 | 0 | 463 | 339 | 43 | 1 | 5 | 3 | 224 | 156 | 15 | 7 | 1 | 6 | 83 | 53 | 82 | 3 | 1 | 9 | 374 | 346 | 8 | 6 | 2 | 12 | 965 | 972 | 9 |
| 2 | 10 | 0 | 634 | 633 | 28 | 3 | 5 | 3 | 130 | 59 | 33 | 0 | 2 | 6 | 1922 | 2034 | 21 | 5 | 1 | 9 | 190 | 146 | 26 | 1 | 3 | 12 | 309 | 285 | 9 |
| 1 | 1 | 1 | 891 | 927 | 3 | 5 | 5 | 3 | 93 | 86 | 93 | 2 | 2 | 6 | 838 | 817 | 4 | 0 | 2 | 9 | 726 | 679 | 5 | 3 | 3 | 12 | 391 | 396 | 10 |
| 3 | 1 | 1 | 77 | 88 | 47 | 0 | 6 | 3 | 451 | 417 | 14 | 4 | 2 | 6 | 1402 | 1425 | 5 | 2 | 2 | 9 | 130 | 93 | 20 | 5 | 3 | 12 | 125 | 117 | 80 |
| 5 | 1 | 1 | 630 | 629 | 6 | 2 | 6 | 3 | 1028 | 1077 | 6 | 6 | 2 | 6 | 370 | 334 | 16 | 4 | 2 | 9 | 238 | 202 | 20 | 0 | 4 | 12 | 1138 | 1140 | 6 |
| 7 | 1 | 1 | 116 | 98 | 63 | 4 | 6 | 3 | 487 | 495 | 11 | 1 | 3 | 6 | 229 | 196 | 9 | 6 | 2 | 9 | 240 | 249 | 30 | 2 | 4 | 12 | 71 | 56 | 70 |
| 0 | 2 | 1 | 582 | 640 | 21 | 1 | 7 | 3 | 448 | 445 | 11 | 3 | 3 | 6 | 319 | 296 | 9 | 1 | 3 | 9 | 37 | 11 | 36 | 4 | 4 | 12 | 1051 | 1050 | 12 |
| 2 | 2 | 1 | 885 | 760 | 5 | 3 | 7 | 3 | 392 | 383 | 13 | 5 | 3 | 6 | 93 | 67 | 93 | 3 | 3 | 9 | 0 | 42 | 1 | 1 | 5 | 12 | 89 | 111 | 89 |
| 4 | 2 | 1 | 305 | 227 | 10 | 5 | 7 | 3 | 256 | 266 | 35 | 0 | 4 | 6 | 1468 | 1503 | 11 | 5 | 3 | 9 | 147 | 121 | 48 | 3 | 5 | 12 | 127 | 117 | 51 |
| 6 | 2 | 1 | 203 | 21 | 26 | 0 | 8 | 3 | 236 | 218 | 40 | 2 | 4 | 6 | 2075 | 2121 | 6 | 0 | 4 | 9 | 869 | 898 | 9 | 5 | 5 | 12 | 170 | 7 | 60 |
| 1 | 3 | 1 | 1080 | 1118 | 4 | 2 | 8 | 3 | 509 | 521 | 11 | 4 | 4 | 6 | 720 | 713 | 6 | 2 | 4 | 9 | 155 | 152 | 21 | 0 | 6 | 12 | 594 | 600 | 13 |
| 3 | 3 | 1 | 1202 | 1176 | 5 | 4 | 8 | 3 | 278 | 258 | 32 | 6 | 4 | 6 | 922 | 952 | 8 | 4 | 4 | 9 | 553 | 543 | 9 | 2 | 6 | 12 | 986 | 991 | 6 |
| 5 | 3 | 1 | 447 | 472 | 9 | 1 | 9 | 3 | 120 | 86 | 91 | 1 | 5 | 6 | 302 | 320 | 8 | 6 | 4 | 9 | 190 | 171 | 54 | 4 | 6 | 12 | 438 | 436 | 14 |
| 7 | 3 | 1 | 552 | 561 | 12 | 3 | 9 | 3 | 117 | 101 | 117 | 3 | 5 | 6 | 266 | 227 | 17 | 1 | 5 | 9 | 334 | 325 | 10 | 1 | 7 | 12 | 390 | 371 | 21 |
| 0 | 4 | 1 | 884 | 850 | 7 | 0 | 10 | 3 | 417 | 390 | 28 | 5 | 5 | 6 | 270 | 233 | 24 | 3 | 5 | 9 | 209 | 183 | 27 | 3 | 7 | 12 | 217 | 209 | 46 |
| 2 | 4 | 1 | 271 | 234 | 10 | 0 | 0 | 4 | 858 | 867 | 4 | 0 | 6 | 6 | 982 | 1055 | 7 | 5 | 5 | 9 | 343 | 290 | 24 | 0 | 8 | 12 | 747 | 698 | 22 |
| 4 | 4 | 1 | 529 | 487 | 7 | 2 | 0 | 4 | 2858 | 2908 | 10 | 2 | 6 | 6 | 770 | 764 | 6 | 0 | 6 | 9 | 349 | 355 | 36 | 2 | 8 | 12 | 715 | 757 | 14 |
| 6 | 4 | 1 | 115 | 15 | 79 | 4 | 0 | 4 | 651 | 622 | 8 | 4 | 6 | 6 | 911 | 910 | 7 | 2 | 6 | 9 | 211 | 203 | 24 | 1 | 1 | 13 | 84 | 48 | 28 |
| 1 | 5 | 1 | 263 | 245 | 13 | 6 | 0 | 4 | 1479 | 1474 | 13 | 1 | 7 | 6 | 40 | 72 | 39 | 4 | 6 | 9 | 78 | 66 | 77 | 3 | 1 | 13 | 307 | 302 | 11 |
| 3 | 5 | 1 | 603 | 608 | 6 | 1 | 1 | 4 | 379 | 317 | 4 | 3 | 7 | 6 | 0 | 6 | 1 | 1 | 7 | 9 | 247 | 239 | 34 | 5 | 1 | 13 | 199 | 194 | 30 |
| 5 | 5 | 1 | 0 | 26 | 1 | 3 | 1 | 4 | 158 | 102 | 18 | 5 | 7 | 6 | 116 | 118 | 116 | 3 | 7 | 9 | 129 | 159 | 101 | 0 | 2 | 13 | 98 | 57 | 44 |
| 0 | 6 | 1 | 315 | 299 | 22 | 5 | 1 | 4 | 420 | 419 | 8 | 0 | 8 | 6 | 295 | 287 | 30 | 0 | 8 | 9 | 222 | 196 | 76 | 2 | 2 | 13 | 189 | 173 | 18 |
| 2 | 6 | 1 | 720 | 670 | 7 | 7 | 1 | 4 | 112 | 32 | 94 | 2 | 8 | 6 | 854 | 851 | 9 | 2 | 8 | 9 | 448 | 474 | 18 | 4 | 2 | 13 | 49 | 59 | 48 |
| 4 | 6 | 1 | 370 | 319 | 15 | 0 | 2 | 4 | 2400 | 2476 | 10 | 4 | 8 | 6 | 373 | 376 | 22 | 1 | 9 | 9 | 0 | 70 | 1 | 6 | 2 | 13 | 95 | 59 | 94 |
| 6 | 6 | 1 | 267 | 255 | 29 | 2 | 2 | 4 | 1110 | 1097 | 4 | 1 | 9 | 6 | 243 | 241 | 40 | 0 | 0 | 10 | 464 | 464 | 5 | 1 | 3 | 13 | 353 | 339 | 8 |
| 1 | 7 | 1 | 389 | 391 | 11 | 4 | 2 | 4 | 1517 | 1519 | 5 | 3 | 9 | 6 | 236 | 212 | 48 | 2 | 0 | 10 | 1340 | 1358 | 14 | 3 | 3 | 13 | 491 | 494 | 8 |
| 3 | 7 | 1 | 244 | 221 | 25 | 6 | 2 | 4 | 527 | 530 | 10 | 0 | 10 | 6 | 600 | 532 | 30 | 4 | 0 | 10 | 584 | 545 | 9 | 5 | 3 | 13 | 127 | 73 | 73 |
| 5 | 7 | 1 | 333 | 295 | 22 | 1 | 3 | 4 | 86 | 90 | 30 | 1 | 1 | 7 | 1164 | 1145 | 3 | 6 | 0 | 10 | 527 | 566 | 14 | 0 | 4 | 13 | 46 | 60 | 45 |
| 0 | 8 | 1 | 290 | 234 | 33 | 3 | 3 | 4 | 492 | 473 | 6 | 3 | 1 | 7 | 358 | 342 | 7 | 1 | 1 | 10 | 160 | 119 | 12 | 2 | 4 | 13 | 341 | 322 | 11 |
| 2 | 8 | 1 | 266 | 256 | 24 | 5 | 3 | 4 | 265 | 247 | 19 | 5 | 1 | 7 | 729 | 747 | 6 | 3 | 1 | 10 | 461 | 458 | 6 | 4 | 4 | 13 | 75 | 19 | 74 |
| 4 | 8 | 1 | 268 | 227 | 29 | 7 | 3 | 4 | 170 | 154 | 58 | 7 | 1 | 7 | 163 | 153 | 43 | 5 | 1 | 10 | 103 | 100 | 82 | 1 | 5 | 13 | 288 | 243 | 15 |
| 1 | 9 | 1 | 232 | 221 | 32 | 0 | 4 | 4 | 659 | 650 | 9 | 0 | 2 | 7 | 1682 | 1679 | 5 | 0 | 2 | 10 | 339 | 356 | 8 | 3 | 5 | 13 | 132 | 91 | 49 |
| 3 | 9 | 1 | 72 | 20 | 72 | 2 | 4 | 4 | 1976 | 2010 | 8 | 2 | 2 | 7 | 567 | 554 | 4 | 2 | 2 | 10 | 1833 | 1828 | 5 | 5 | 5 | 13 | 298 | 294 | 30 |
| 0 | 10 | 1 | 194 | 109 | 93 | 4 | 4 | 4 | 434 | 411 | 8 | 4 | 2 | 7 | 740 | 736 | 5 | 4 | 2 | 10 | 300 | 248 | 17 | 0 | 6 | 13 | 282 | 247 | 28 |
| 2 | 10 | 1 | 84 | 4 | 83 | 6 | 4 | 4 | 995 | 1020 | 8 | 6 | 2 | 7 | 335 | 310 | 19 | 6 | 2 | 10 | 1057 | 1088 | 8 | 2 | 6 | 13 | 328 | 323 | 14 |
| 0 | 0 | 2 | 2353 | 2225 | 10 | 1 | 5 | 4 | 250 | 266 | 12 | 1 | 3 | 7 | 723 | 710 | 7 | 1 | 3 | 10 | 207 | 165 | 12 | 4 | 6 | 13 | 221 | 232 | 32 |
| 2 | 0 | 2 | 968 | 1024 | 6 | 3 | 5 | 4 | 412 | 400 | 9 | 3 | 3 | 7 | 198 | 181 | 18 | 3 | 3 | 10 | 265 | 240 | 16 | 1 | 7 | 13 | 210 | 221 | 47 |
| 4 | 0 | 2 | 1230 | 1247 | 7 | 5 | 5 | 4 | 41 | 63 | 41 | 5 | 3 | 7 | 394 | 387 | 13 | 5 | 3 | 10 | 260 | 271 | 27 | 3 | 7 | 13 | 136 | 101 | 99 |
| 6 | 0 | 2 | 413 | 391 | 14 | 0 | 6 | 4 | 1251 | 1274 | 9 | 0 | 4 | 7 | 472 | 468 | 7 | 0 | 4 | 10 | 1817 | 1845 | 7 | 0 | 8 | 13 | 422 | 386 | 42 |
| 1 | 1 | 2 | 220 | 183 | 6 | 2 | 6 | 4 | 476 | 455 | 9 | 2 | 4 | 7 | 930 | 937 | 5 | 2 | 4 | 10 | 335 | 317 | 9 | | | | | | |

Table 1. Observed and calculated structure factors for ercitate

| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
|---|---|----|------|------|-----|---|---|----|------|------|-----|---|---|----|------|------|-----|---|---|----|------|------|-----|---|---|----|------|------|-----|
| 4 | 2 | 15 | 319 | 282 | 16 | 4 | 2 | 16 | 1053 | 1038 | 7 | 2 | 4 | 17 | 170 | 159 | 28 | 0 | 6 | 18 | 710 | 707 | 14 | 3 | 3 | 20 | 19 | 32 | 19 |
| 1 | 3 | 15 | 918 | 924 | 12 | 1 | 3 | 16 | 137 | 141 | 31 | 4 | 4 | 17 | 0 | 17 | 1 | 2 | 6 | 18 | 506 | 493 | 14 | 0 | 4 | 20 | 1071 | 1090 | 22 |
| 3 | 3 | 15 | 675 | 682 | 6 | 3 | 3 | 16 | 198 | 153 | 22 | 1 | 5 | 17 | 0 | 68 | 1 | 1 | 1 | 19 | 288 | 236 | 15 | 2 | 4 | 20 | 541 | 545 | 11 |
| 5 | 3 | 15 | 613 | 651 | 11 | 5 | 3 | 16 | 222 | 229 | 34 | 3 | 5 | 17 | 128 | 157 | 54 | 3 | 1 | 19 | 389 | 423 | 14 | 1 | 5 | 20 | 142 | 81 | 58 |
| 0 | 4 | 15 | 174 | 103 | 39 | 0 | 4 | 16 | 380 | 374 | 15 | 0 | 6 | 17 | 527 | 544 | 17 | 0 | 2 | 19 | 437 | 412 | 19 | 1 | 1 | 21 | 461 | 448 | 13 |
| 2 | 4 | 15 | 374 | 341 | 11 | 2 | 4 | 16 | 1049 | 1049 | 5 | 2 | 6 | 17 | 74 | 88 | 74 | 2 | 2 | 19 | 373 | 339 | 12 | 3 | 1 | 21 | 529 | 541 | 12 |
| 4 | 4 | 15 | 73 | 63 | 72 | 4 | 4 | 16 | 331 | 318 | 19 | 1 | 7 | 17 | 146 | 65 | 105 | 4 | 2 | 19 | 375 | 328 | 26 | 0 | 2 | 21 | 77 | 21 | 76 |
| 1 | 5 | 15 | 609 | 641 | 7 | 1 | 5 | 16 | 150 | 139 | 33 | 0 | 0 | 18 | 623 | 591 | 13 | 1 | 3 | 19 | 197 | 182 | 25 | 2 | 2 | 21 | 235 | 206 | 25 |
| 3 | 5 | 15 | 418 | 417 | 12 | 3 | 5 | 16 | 0 | 7 | 1 | 2 | 0 | 18 | 287 | 208 | 24 | 3 | 3 | 19 | 0 | 12 | 1 | 1 | 3 | 21 | 169 | 147 | 53 |
| 0 | 6 | 15 | 0 | 16 | 1 | 0 | 6 | 16 | 1000 | 1061 | 10 | 4 | 0 | 18 | 590 | 572 | 16 | 0 | 4 | 19 | 154 | 58 | 57 | 0 | 4 | 21 | 279 | 279 | 36 |
| 2 | 6 | 15 | 435 | 406 | 17 | 2 | 6 | 16 | 267 | 230 | 26 | 1 | 1 | 18 | 287 | 280 | 14 | 2 | 4 | 19 | 376 | 359 | 14 | 0 | 0 | 22 | 473 | 503 | 34 |
| 1 | 7 | 15 | 171 | 203 | 68 | 1 | 7 | 16 | 89 | 116 | 89 | 3 | 1 | 18 | 116 | 104 | 61 | 1 | 5 | 19 | 144 | 65 | 47 | 2 | 0 | 22 | 372 | 366 | 22 |
| 0 | 8 | 15 | 187 | 66 | 187 | 1 | 1 | 17 | 81 | 7 | 80 | 0 | 2 | 18 | 695 | 673 | 11 | 0 | 6 | 19 | 442 | 395 | 23 | 1 | 1 | 22 | 327 | 327 | 19 |
| 0 | 0 | 16 | 230 | 159 | 57 | 3 | 1 | 17 | 72 | 61 | 72 | 2 | 2 | 18 | 814 | 844 | 8 | 0 | 0 | 20 | 1039 | 1034 | 21 | 0 | 2 | 22 | 219 | 256 | 53 |
| 2 | 0 | 16 | 2072 | 2107 | 11 | 5 | 1 | 17 | 127 | 106 | 69 | 4 | 2 | 18 | 567 | 553 | 10 | 2 | 0 | 20 | 290 | 243 | 24 | 2 | 2 | 22 | 935 | 947 | 9 |
| 4 | 0 | 16 | 175 | 112 | 41 | 0 | 2 | 17 | 377 | 367 | 11 | 1 | 3 | 18 | 203 | 210 | 22 | 4 | 0 | 20 | 927 | 956 | 18 | 1 | 3 | 22 | 58 | 64 | 57 |
| 1 | 1 | 16 | 105 | 72 | 35 | 2 | 2 | 17 | 344 | 355 | 11 | 3 | 3 | 18 | 363 | 341 | 12 | 1 | 1 | 20 | 173 | 171 | 35 | 1 | 1 | 23 | 326 | 333 | 21 |
| 3 | 1 | 16 | 197 | 173 | 20 | 4 | 2 | 17 | 137 | 103 | 47 | 0 | 4 | 18 | 938 | 953 | 9 | 3 | 1 | 20 | 141 | 90 | 58 | 0 | 2 | 23 | 95 | 141 | 95 |
| 5 | 1 | 16 | 186 | 169 | 40 | 1 | 3 | 17 | 625 | 627 | 6 | 2 | 4 | 18 | 919 | 905 | 6 | 0 | 2 | 20 | 676 | 706 | 14 | | | | | | |
| 0 | 2 | 16 | 1323 | 1298 | 6 | 3 | 3 | 17 | 622 | 628 | 7 | 1 | 5 | 18 | 419 | 425 | 11 | 2 | 2 | 20 | 801 | 808 | 7 | | | | | | |
| 2 | 2 | 16 | 551 | 539 | 6 | 0 | 4 | 17 | 0 | 48 | 1 | 3 | 5 | 18 | 309 | 308 | 18 | 1 | 3 | 20 | 43 | 88 | 42 | | | | | | |

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