AM-95-573

# Artroeite, $PbAlF_3(OH)_2$, a new mineral from the Grand Reef mine, Graham County, Arizona: Description and crystal structure

Anthony R. Kampf, Eugene E. Foord

For deposit: Table 6

American Mineralogist, 80, 1-2, 179-183.

Table 6. Observed and calculated structure factors for artroeite.



| K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | 4 | 1 | 583 | 577 | -8 | 1 | 347 | 347 | -3 | 3 | 297 | 294 | 2 | -6 | 369 | 368 | 6 | 2 | 187 | 188 | -5 | 0 | 75 | 71 | -1 | 6 | 162 | 159 |
| **** | H = | 0 | **** | 4 | 2 | 287 | 280 | -8 | 2 | 190 | 182 | -3 | 4 | 391 | 401 | 2 | -5 | 172 | 167 | 6 | 3 | 244 | 241 | -5 | 1 | 355 | 342 | 0 | -7 | 75 | 77 |
| 0 | 1 | 328 | 312 | 4 | 3 | 326 | 332 | -8 | 3 | 242 | 245 | -3 | 5 | 89 | 93 | 2 | -4 | 349 | 345 | 7 | -4 | 137 | 140 | -5 | 2 | 423 | 427 | 0 | -6 | 234 | 232 |
| 0 | 2 | 598 | 581 | 4 | 4 | 305 | 310 | -7 | -4 | 127 | 129 | -3 | 6 | 284 | 283 | 2 | -3 | 546 | 575 | 7 | -3 | 256 | 257 | -5 | 3 | 169 | 159 | 0 | -5 | 370 | 372 |
| 0 | 3 | 641 | 635 | 4 | 5 | 41 | 32 | -7 | -3 | 180 | 179 | -2 | -5 | 387 | 387 | 2 | -2 | 103 | 106 | 7 | -2 | 61 | 59 | -5 | 4 | 375 | 384 | 0 | -4 | 121 | 119 |
| 0 | 4 | 103 | 99 | 5 | -5 | 257 | 258 | -7 | -2 | 307 | 303 | -2 | -4 | 347 | 343 | 2 | -1 | 684 | 717 | 7 | -1 | 367 | 372 | -5 | 5 | 102 | 108 | 0 | -3 | 586 | 598 |
| 0 | 5 | 401 | 392 | 5 | -4 | 212 | 210 | -7 | -1 | 65 | 55 | -2 | -3 | 313 | 303 | 2 | 0 | 144 | 147 | 7 | 0 | 149 | 145 | -4 | -6 | 179 | 178 | 0 | -2 | 40 | 27 |
| 0 | 6 | 52 | 43 | 5 | -3 | 227 | 232 | -7 | 0 | 404 | 397 | -2 | -2 | 933 | 999 | 2 | 1 | 525 | 521 | 7 | 1 | 263 | 266 | -4 | -5 | 228 | 225 | 0 | -1 | 538 | 562 |
| 1 | -6 | 277 | 269 | 5 | -2 | 534 | 538 | -7 | 1 | 187 | 181 | -2 | -1 | 193 | 183 | 2 | 2 | 516 | 524 | 7 | 2 | 312 | 319 | -4 | -4 | 462 | 468 | 0 | 0 | 630 | 709 |
| 1 | -5 | 208 | 205 | 5 | -1 | 35 | 32 | -7 | 2 | 252 | 252 | -2 | 0 | 732 | 732 | 2 | 3 | 176 | 173 | 7 | 3 | 42 | 41 | -4 | -3 | 64 | 60 | 0 | 1 | 428 | 429 |
| 1 | -4 | 226 | 218 | 5 | 0 | 441 | 432 | -7 | 3 | 261 | 261 | -2 | 1 | 725 | 730 | 2 | 4 | 390 | 394 | 8 | -3 | 109 | 106 | -4 | -2 | 589 | 589 | 0 | 2 | 594 | 582 |
| 1 | -3 | 481 | 480 | 5 | 1 | 297 | 293 | -7 | 4 | 71 | 74 | -2 | 2 | 232 | 231 | 2 | 5 | 113 | 111 | 8 | -2 | 266 | 273 | -4 | -1 | 463 | 456 | 0 | 3 | 137 | 133 |
| 1 | -2 | 100 | 91 | 5 | 2 | 285 | 280 | -6 | -5 | 164 | 163 | -2 | 3 | 573 | 592 | 2 | 6 | 172 | 170 | 8 | -1 | 223 | 222 | -4 | 0 | 359 | 344 | 0 | 4 | 275 | 279 |
| 1 | -1 | 586 | 639 | 5 | 3 | 299 | 305 | -6 | -4 | 227 | 223 | -2 | 5 | 300 | 298 | 3 | -6 | 130 | 131 | 8 | 0 | 135 | 137 | -4 | 1 | 613 | 600 | 0 | 5 | 195 | 197 |
| 1 | 0 | 211 | 201 | 5 | 4 | 106 | 105 | -6 | -3 | 348 | 355 | -2 | 6 | 198 | 205 | 3 | -5 | 223 | 218 | 8 | 1 | 258 | 261 | -4 | 3 | 435 | 447 | 0 | 6 | 118 | 120 |
| 1 | 1 | 489 | 487 | 5 | 5 | 255 | 254 | -6 | -1 | 462 | 465 | -1 | -6 | 218 | 210 | 3 | -4 | 452 | 472 | 8 | 2 | 42 | 41 | -4 | 4 | 223 | 227 | 1 | -7 | 154 | 163 |
| 1 | 2 | 552 | 533 | 6 | -5 | 210 | 214 | -6 | 0 | 346 | 348 | -1 | -5 | 290 | 282 | 3 | -3 | 137 | 134 | | | | | -4 | 5 | 190 | 189 | 1 | -6 | 260 | 269 |
| 1 | 3 | 250 | 242 | 6 | -4 | 220 | 223 | -6 | 1 | 369 | 357 | -1 | -4 | 78 | 74 | 3 | -2 | 484 | 489 | **** | H = | 2 | **** | -3 | -6 | 63 | 65 | 1 | -5 | 138 | 130 |
| 1 | 4 | 376 | 370 | 6 | -3 | 386 | 395 | -6 | 2 | 410 | 410 | -1 | -3 | 506 | 492 | 3 | -1 | 364 | 346 | -9 | -2 | 235 | 232 | -3 | -5 | 294 | 293 | 1 | -4 | 426 | 424 |
| 1 | 5 | 62 | 58 | 6 | -2 | 35 | 34 | -6 | 3 | 38 | 30 | -1 | -2 | 218 | 206 | 3 | 0 | 505 | 495 | -9 | -1 | 105 | 101 | -3 | -4 | 98 | 94 | 1 | -3 | 191 | 181 |
| 1 | 6 | 246 | 240 | 6 | -1 | 431 | 437 | -6 | 4 | 354 | 351 | -1 | -1 | 569 | 573 | 3 | 1 | 469 | 462 | -9 | 0 | 216 | 221 | -3 | -3 | 430 | 432 | 1 | -2 | 564 | 603 |
| 2 | -6 | 99 | 93 | 6 | 0 | 357 | 358 | -6 | 5 | 148 | 148 | -1 | 0 | 420 | 403 | 3 | 2 | 276 | 276 | -9 | 1 | 199 | 204 | -3 | -2 | 192 | 188 | 1 | -1 | 510 | 530 |
| 2 | -5 | 336 | 322 | 6 | 1 | 274 | 277 | -5 | -5 | 129 | 135 | -1 | 1 | 304 | 301 | 3 | 3 | 444 | 441 | -9 | 2 | 113 | 119 | -3 | -1 | 301 | 284 | 1 | 0 | 461 | 480 |
| 2 | -4 | 402 | 401 | 6 | 2 | 341 | 338 | -5 | -4 | 273 | 274 | -1 | 2 | 562 | 596 | 3 | 4 | 131 | 131 | -8 | -3 | 280 | 287 | -3 | 0 | 693 | 678 | 1 | 1 | 656 | 677 |
| 2 | -3 | 171 | 168 | 6 | 3 | 58 | 53 | -5 | -3 | 49 | 46 | -1 | 3 | 68 | 21 | 3 | 5 | 315 | 313 | -8 | -2 | 181 | 183 | -3 | 1 | 137 | 130 | 1 | 2 | 149 | 145 |
| 2 | -2 | 883 | 978 | 6 | 4 | 258 | 260 | -5 | -2 | 477 | 479 | -1 | 4 | 426 | 416 | 4 | -6 | 188 | 187 | -8 | -1 | 285 | 284 | -3 | 2 | 564 | 568 | 1 | 3 | 552 | 554 |
| 2 | -1 | 348 | 339 | 7 | -4 | 295 | 293 | -5 | -1 | 269 | 261 | -1 | 5 | 205 | 207 | 4 | -5 | 341 | 351 | -8 | 0 | 293 | 294 | -3 | 3 | 245 | 246 | 1 | 4 | 288 | 294 |
| 2 | 0 | 624 | 624 | 7 | -3 | 48 | 48 | -5 | 0 | 268 | 262 | -1 | 6 | 172 | 171 | 4 | -3 | 464 | 471 | -8 | 1 | 40 | 40 | -3 | 4 | 235 | 245 | 1 | 5 | 137 | 139 |
| 2 | 1 | 805 | 822 | 7 | -2 | 319 | 323 | -5 | 1 | 416 | 411 | 0 | -6 | 228 | 229 | 4 | -2 | 334 | 331 | -8 | 2 | 351 | 358 | -3 | 5 | 306 | 316 | 2 | -5 | 375 | 384 |
| 2 | 2 | 100 | 96 | 7 | -1 | 229 | 226 | -5 | 2 | 43 | 37 | 0 | -5 | 155 | 148 | 4 | -1 | 413 | 403 | -8 | 3 | 131 | 129 | -2 | -6 | 380 | 372 | 2 | -4 | 186 | 181 |
| 2 | 3 | 568 | 573 | 7 | 0 | 206 | 202 | -5 | 3 | 420 | 411 | 0 | -4 | 681 | 701 | 4 | 0 | 500 | 491 | -7 | -4 | 247 | 252 | -2 | -5 | 61 | 69 | 2 | -3 | 367 | 380 |
| 2 | 4 | 140 | 139 | 7 | 1 | 303 | 307 | -5 | 4 | 69 | 62 | 0 | -3 | 161 | 150 | 4 | 1 | 31 | 18 | -7 | -3 | 145 | 150 | -2 | -4 | 426 | 415 | 2 | -2 | 580 | 596 |
| 2 | 5 | 261 | 261 | 7 | 2 | 51 | 53 | -5 | 5 | 230 | 230 | 0 | -2 | 575 | 572 | 4 | 2 | 455 | 460 | -7 | -2 | 201 | 206 | -2 | -3 | 489 | 480 | 2 | -1 | 171 | 165 |
| 2 | 6 | 233 | 231 | 7 | 3 | 295 | 300 | -4 | -6 | 135 | 133 | 0 | -1 | 716 | 840 | 4 | 3 | 188 | 185 | -7 | -1 | 292 | 283 | -2 | -2 | 295 | 279 | 2 | 0 | 628 | 643 |
| 3 | -6 | 84 | 86 | 8 | -3 | 281 | 286 | -4 | -5 | 307 | 310 | 0 | 0 | 200 | 214 | 4 | 4 | 203 | 205 | -7 | 0 | 96 | 92 | -2 | -1 | 749 | 742 | 2 | 1 | 275 | 277 |
| 3 | -5 | 337 | 336 | 8 | -2 | 300 | 299 | -4 | -3 | 503 | 506 | 0 | 1 | 809 | 832 | 4 | 5 | 188 | 185 | -7 | 1 | 349 | 348 | -2 | 0 | 146 | 127 | 2 | 2 | 327 | 322 |
| 3 | -3 | 448 | 448 | 8 | -1 | 147 | 152 | -4 | -2 | 439 | 434 | 0 | 2 | 27 | 23 | 5 | -6 | 269 | 261 | -7 | 2 | 52 | 47 | -2 | 1 | 614 | 602 | 2 | 3 | 300 | 303 |
| 3 | -2 | 269 | 262 | 8 | 0 | 323 | 318 | -4 | -1 | 418 | 412 | 0 | 3 | 452 | 439 | 5 | -4 | 306 | 303 | -7 | 3 | 291 | 298 | -2 | 2 | 468 | 480 | 2 | 4 | 99 | 98 |
| 3 | -1 | 378 | 362 | 8 | 1 | 108 | 107 | -4 | 0 | 770 | 774 | 0 | 4 | 406 | 395 | 5 | -3 | 230 | 232 | -7 | 4 | 231 | 229 | -2 | 3 | 322 | 332 | 2 | 5 | 210 | 209 |
| 3 | 0 | 779 | 776 | 8 | 2 | 229 | 235 | -4 | 1 | 142 | 137 | 0 | 5 | 187 | 183 | 5 | -2 | 313 | 315 | -6 | -5 | 272 | 271 | -2 | 4 | 393 | 394 | 3 | -6 | 226 | 224 |
| 3 | 1 | 176 | 167 | 9 | -2 | 98 | 103 | -4 | 2 | 568 | 570 | 0 | 6 | 268 | 265 | 5 | -1 | 388 | 386 | -6 | -4 | 216 | 219 | -2 | 6 | 190 | 190 | 3 | -5 | 154 | 151 |
| 3 | 2 | 446 | 437 | 9 | -1 | 238 | 240 | -4 | 3 | 371 | 365 | 1 | -6 | 41 | 36 | 5 | 0 | 200 | 197 | -6 | -3 | 303 | 307 | -1 | -7 | 208 | 212 | 3 | -4 | 323 | 330 |
| 3 | 3 | 223 | 215 | 9 | 1 | 251 | 260 | -4 | 4 | 193 | 194 | 1 | -5 | 350 | 350 | 5 | 1 | 480 | 481 | -6 | -2 | 421 | 425 | -1 | -6 | 94 | 94 | 3 | -3 | 346 | 354 |
| 3 | 4 | 288 | 291 | | | | | -4 | 5 | 308 | 312 | 1 | -4 | 188 | 182 | 5 | 2 | 161 | 164 | -6 | -1 | 32 | 34 | -1 | -5 | 304 | 299 | 3 | -2 | 336 | 338 |
| 3 | 5 | 225 | 225 | **** | H = | 1 | **** | -3 | -6 | 205 | 212 | 1 | -3 | 400 | 386 | 5 | 3 | 354 | 354 | -6 | 0 | 540 | 543 | -1 | -4 | 327 | 311 | 3 | -1 | 600 | 601 |
| 3 | 6 | 124 | 119 | -9 | -1 | 171 | 170 | -3 | -5 | 123 | 117 | 1 | -2 | 614 | 667 | 5 | 4 | 283 | 286 | -6 | 1 | 283 | 286 | -1 | -3 | 228 | 214 | 3 | 0 | 206 | 204 |
| 4 | -6 | 253 | 253 | -9 | 0 | 250 | 251 | -3 | -4 | 373 | 377 | 1 | -1 | 251 | 250 | 6 | -5 | 279 | 283 | -6 | 2 | 285 | 285 | -1 | -2 | 692 | 682 | 3 | 1 | 659 | 671 |
| 4 | -5 | 65 | 55 | -9 | 1 | 97 | 92 | -3 | -3 | 301 | 298 | 1 | 0 | 614 | 650 | 6 | -4 | 287 | 286 | -6 | 3 | 347 | 347 | -1 | -1 | 92 | 80 | 3 | 2 | 415 | 413 |
| 4 | -4 | 447 | 452 | -9 | 2 | 260 | 251 | -3 | -2 | 158 | 154 | 1 | 1 | 271 | 263 | 6 | -3 | 227 | 230 | -6 | 5 | 267 | 268 | -1 | 0 | 720 | 714 | 3 | 3 | 144 | 138 |
| 4 | -3 | 300 | 298 | -8 | -3 | 130 | 134 | -3 | -1 | 508 | 507 | 1 | 2 | 527 | 517 | 6 | -2 | 399 | 389 | -5 | -5 | 163 | 167 | -1 | 1 | 516 | 479 | 3 | 4 | 363 | 363 |
| 4 | -2 | 422 | 426 | -8 | -2 | 265 | 262 | -3 | 0 | 103 | 98 | 1 | 3 | 369 | 367 | 6 | -1 | 115 | 114 | -5 | -4 | 124 | 130 | -1 | 2 | 365 | 351 | 3 | 5 | 80 | 83 |
| 4 | -1 | 624 | 613 | -8 | -1 | 315 | 313 | -3 | 1 | 587 | 576 | 1 | 4 | 243 | 242 | 6 | 0 | 402 | 402 | -5 | -3 | 316 | 319 | -1 | 3 | 525 | 518 | 4 | -6 | 192 | 183 |
| 4 | 0 | 60 | 48 | -8 | 0 | 61 | 57 | -3 | 2 | 126 | 123 | 1 | 5 | 317 | 320 | 6 | 1 | 237 | 235 | -5 | -1 | 453 | 444 | -1 | 5 | 342 | 328 | 4 | -5 | 224 | 231 |

Table 6. Observed and calculated structure factors for artroeite.



| K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | -4 | 376 | 391 | -8 | 3 | 294 | 293 | -2 | -6 | 114 | 108 | 2 | 1 | 406 | 406 | -9 | -1 | 137 | 134 | -3 | 1 | 463 | 457 | 2 | -4 | 85 | 86 | -7 | -2 | 146 | 149 |
| 4 | -3 | 48 | 38 | -7 | -4 | 47 | 38 | -2 | -5 | 373 | 366 | 2 | 2 | 77 | 78 | -9 | 0 | 296 | 298 | -3 | 2 | 491 | 489 | 2 | -3 | 404 | 414 | -7 | -1 | 350 | 351 |
| 4 | -2 | 511 | 521 | -7 | -3 | 262 | 263 | -2 | -3 | 451 | 440 | 2 | 3 | 290 | 293 | -9 | 1 | 46 | 50 | -3 | 3 | 55 | 60 | 2 | -2 | 122 | 121 | -7 | 0 | 87 | 86 |
| 4 | -1 | 316 | 310 | -7 | -2 | 62 | 60 | -2 | -2 | 527 | 515 | 2 | 4 | 182 | 178 | -8 | -3 | 234 | 241 | -3 | 4 | 338 | 345 | 2 | -1 | 405 | 416 | -7 | 1 | 334 | 337 |
| 4 | 0 | 296 | 297 | -7 | -1 | 311 | 312 | -2 | -1 | 453 | 429 | 2 | 5 | 112 | 114 | -8 | -2 | 44 | 38 | -3 | 5 | 147 | 155 | 2 | 0 | 337 | 342 | -7 | 2 | 281 | 282 |
| 4 | 1 | 371 | 374 | -7 | 0 | 311 | 311 | -2 | 0 | 638 | 623 | 3 | -6 | 137 | 133 | -8 | -1 | 345 | 350 | -2 | -6 | 254 | 256 | 2 | 1 | 190 | 190 | -6 | -5 | 157 | 152 |
| 4 | 2 | 33 | 24 | -7 | 1 | 173 | 167 | -2 | 1 | 118 | 108 | 3 | -5 | 312 | 315 | -8 | 0 | 82 | 80 | -2 | -5 | 196 | 186 | 2 | 2 | 363 | 370 | -6 | -4 | 260 | 263 |
| 4 | 3 | 312 | 317 | -7 | 2 | 385 | 390 | -2 | 2 | 375 | 369 | 3 | -4 | 117 | 118 | -8 | 1 | 217 | 220 | -2 | -4 | 431 | 427 | 2 | 4 | 221 | 222 | -6 | -3 | 42 | 37 |
| 4 | 4 | 64 | 65 | -7 | 3 | 88 | 87 | -2 | 3 | 239 | 246 | 3 | -3 | 525 | 533 | -8 | 2 | 215 | 217 | -2 | -3 | 162 | 159 | 3 | -6 | 211 | 210 | -6 | -2 | 311 | 318 |
| 5 | -6 | 141 | 142 | -7 | 4 | 211 | 216 | -2 | 4 | 216 | 224 | 3 | -2 | 389 | 394 | -7 | -4 | 231 | 234 | -2 | -2 | 373 | 356 | 3 | -5 | 79 | 80 | -6 | -1 | 101 | 101 |
| 5 | -5 | 207 | 213 | -6 | -4 | 345 | 362 | -2 | 5 | 169 | 171 | 3 | -1 | 179 | 183 | -7 | -3 | 117 | 118 | -2 | -1 | 390 | 378 | 3 | -4 | 373 | 377 | -6 | 0 | 245 | 248 |
| 5 | -4 | 128 | 126 | -6 | -3 | 217 | 219 | -1 | -7 | 88 | 88 | 3 | 0 | 542 | 552 | -7 | -2 | 371 | 378 | -2 | 0 | 312 | 302 | 3 | -3 | 129 | 124 | -6 | 1 | 234 | 238 |
| 5 | -3 | 390 | 392 | -6 | -2 | 303 | 302 | -1 | -6 | 294 | 283 | 3 | 1 | 126 | 126 | -7 | -1 | 131 | 130 | -2 | 1 | 295 | 278 | 3 | -2 | 410 | 416 | -6 | 2 | 143 | 145 |
| 5 | -2 | 165 | 154 | -6 | -1 | 423 | 419 | -1 | -4 | 447 | 453 | 3 | 2 | 401 | 409 | -7 | 0 | 283 | 287 | -2 | 2 | 41 | 39 | 3 | -1 | 284 | 283 | -6 | 3 | 253 | 251 |
| 5 | -1 | 456 | 460 | -6 | 1 | 471 | 477 | -1 | -3 | 382 | 358 | 3 | 3 | 227 | 229 | -7 | 1 | 304 | 307 | -2 | 3 | 348 | 369 | 3 | 0 | 175 | 175 | -5 | -5 | 268 | 269 |
| 5 | 0 | 413 | 416 | -6 | 2 | 163 | 163 | -1 | -2 | 444 | 417 | 3 | 4 | 123 | 122 | -7 | 2 | 141 | 142 | -2 | 4 | 112 | 110 | 3 | 1 | 462 | 474 | -5 | -4 | 139 | 135 |
| 5 | 1 | 102 | 104 | -6 | 3 | 236 | 228 | -1 | -1 | 745 | 753 | 4 | -6 | 284 | 286 | -7 | 3 | 276 | 284 | -2 | 5 | 189 | 186 | 3 | 2 | 69 | 67 | -5 | -3 | 379 | 375 |
| 5 | 2 | 394 | 401 | -6 | 4 | 256 | 254 | -1 | 1 | 653 | 706 | 4 | -5 | 187 | 190 | -6 | -5 | 234 | 233 | -1 | -7 | 128 | 128 | 3 | 3 | 264 | 266 | -5 | -2 | 169 | 169 |
| 5 | 3 | 118 | 124 | -5 | -5 | 242 | 247 | -1 | 2 | 384 | 377 | 4 | -4 | 242 | 245 | -6 | -3 | 375 | 383 | -1 | -6 | 184 | 182 | 4 | -5 | 304 | 303 | -5 | -1 | 439 | 438 |
| 5 | 4 | 218 | 215 | -5 | -4 | 98 | 95 | -1 | 3 | 312 | 302 | 4 | -3 | 377 | 381 | -6 | -2 | 162 | 160 | -1 | -5 | 360 | 363 | 4 | -4 | 120 | 110 | -5 | 0 | 442 | 441 |
| 6 | -5 | 60 | 64 | -5 | -3 | 243 | 247 | -1 | 4 | 395 | 388 | 4 | -2 | 37 | 22 | -6 | -1 | 270 | 272 | -1 | -4 | 40 | 34 | 4 | -3 | 256 | 251 | -5 | 1 | 142 | 137 |
| 6 | -4 | 319 | 327 | -5 | -2 | 457 | 455 | 0 | -7 | 239 | 244 | 4 | -1 | 464 | 473 | -6 | 0 | 362 | 362 | -1 | -3 | 570 | 582 | 4 | -2 | 318 | 321 | -5 | 2 | 391 | 391 |
| 6 | -3 | 234 | 235 | -5 | -1 | 154 | 150 | 0 | -6 | 61 | 63 | 4 | 0 | 145 | 145 | -6 | 1 | 89 | 84 | -1 | -2 | 351 | 351 | 4 | -1 | 135 | 128 | -5 | 3 | 174 | 175 |
| 6 | -2 | 228 | 216 | -5 | 0 | 550 | 547 | 0 | -5 | 286 | 289 | 4 | 1 | 262 | 261 | -6 | 2 | 325 | 327 | -1 | -1 | 431 | 438 | 4 | 0 | 369 | 379 | -4 | -6 | 251 | 243 |
| 6 | -1 | 358 | 356 | -5 | 1 | 219 | 215 | 0 | -4 | 462 | 467 | 4 | 2 | 274 | 277 | -6 | 3 | 68 | 69 | -1 | 0 | 609 | 632 | 4 | 1 | 40 | 40 | -4 | -5 | 52 | 49 |
| 6 | 0 | 47 | 49 | -5 | 2 | 291 | 289 | 0 | -3 | 259 | 244 | 4 | 3 | 91 | 92 | -6 | 4 | 196 | 198 | -1 | 2 | 506 | 526 | 4 | 2 | 245 | 245 | -4 | -4 | 277 | 278 |
| 6 | 1 | 362 | 360 | -5 | 3 | 378 | 374 | 0 | -2 | 604 | 613 | 4 | 4 | 240 | 236 | -5 | -6 | 234 | 227 | -1 | 3 | 229 | 232 | 4 | 3 | 197 | 195 | -4 | -3 | 211 | 211 |
| 6 | 2 | 139 | 136 | -5 | 4 | 116 | 112 | 0 | -1 | 292 | 297 | 5 | -5 | 255 | 251 | -5 | -5 | 78 | 77 | -1 | 4 | 209 | 203 | 5 | -5 | 109 | 118 | -4 | -2 | 256 | 253 |
| 6 | 3 | 133 | 138 | -5 | 5 | 236 | 240 | 0 | 0 | 354 | 367 | 5 | -4 | 293 | 299 | -5 | -4 | 366 | 372 | -1 | 5 | 259 | 258 | 5 | -4 | 241 | 235 | -4 | -1 | 296 | 285 |
| 7 | -4 | 121 | 117 | -4 | -6 | 252 | 252 | 0 | 1 | 406 | 420 | 5 | -3 | 72 | 69 | -5 | -3 | 192 | 191 | 0 | -7 | 97 | 95 | 5 | -3 | 280 | 279 | -4 | 0 | 94 | 95 |
| 7 | -3 | 219 | 215 | -4 | -5 | 225 | 227 | 0 | 2 | 220 | 218 | 5 | -2 | 407 | 406 | -5 | -2 | 305 | 297 | 0 | -6 | 308 | 317 | 5 | -2 | 103 | 102 | -4 | 1 | 399 | 392 |
| 7 | -2 | 334 | 327 | -4 | -4 | 221 | 221 | 0 | 3 | 267 | 262 | 5 | -1 | 158 | 156 | -5 | -1 | 479 | 488 | 0 | -5 | 173 | 174 | 5 | -1 | 401 | 401 | -4 | 2 | 104 | 105 |
| 7 | -1 | 62 | 47 | -4 | -3 | 450 | 450 | 0 | 5 | 250 | 253 | 5 | 0 | 324 | 319 | -5 | 0 | 176 | 171 | 0 | -4 | 298 | 292 | 5 | 0 | 147 | 144 | -4 | 3 | 263 | 257 |
| 7 | 0 | 331 | 328 | -4 | -2 | 38 | 38 | 1 | -7 | 65 | 61 | 5 | 1 | 285 | 283 | -5 | 1 | 437 | 428 | 0 | -3 | 424 | 424 | 5 | 1 | 254 | 255 | -4 | 4 | 184 | 185 |
| 7 | 1 | 148 | 145 | -4 | -1 | 565 | 569 | 1 | -6 | 249 | 249 | 5 | 2 | 109 | 112 | -5 | 2 | 176 | 173 | 0 | -2 | 207 | 205 | 5 | 2 | 267 | 260 | -3 | -6 | 60 | 66 |
| 7 | 2 | 181 | 186 | -4 | 0 | 349 | 341 | 1 | -5 | 235 | 236 | 5 | 3 | 305 | 302 | -5 | 3 | 322 | 325 | 0 | -1 | 374 | 381 | 6 | -4 | 224 | 223 | -3 | -5 | 323 | 318 |
| 8 | -3 | 261 | 262 | -4 | 1 | 379 | 367 | 1 | -4 | 295 | 300 | 6 | -5 | 229 | 244 | -5 | 4 | 284 | 287 | 0 | 0 | 79 | 76 | 6 | -3 | 59 | 48 | -3 | -4 | 196 | 191 |
| 8 | -2 | 47 | 45 | -4 | 2 | 452 | 451 | 1 | -3 | 525 | 533 | 6 | -4 | 45 | 25 | -4 | -5 | 310 | 303 | 0 | 1 | 450 | 472 | 6 | -2 | 273 | 272 | -3 | -3 | 390 | 389 |
| 8 | -1 | 279 | 284 | -4 | 3 | 40 | 27 | 1 | -2 | 103 | 104 | 6 | -3 | 355 | 352 | -4 | -4 | 250 | 248 | 0 | 2 | 226 | 226 | 6 | -1 | 54 | 56 | -3 | -2 | 501 | 498 |
| 8 | 0 | 178 | 173 | -4 | 4 | 281 | 280 | 1 | -1 | 751 | 822 | 6 | -2 | 167 | 160 | -4 | -3 | 264 | 264 | 0 | 3 | 218 | 213 | 6 | 0 | 208 | 213 | -3 | -1 | 113 | 113 |
| 8 | 1 | 110 | 113 | -4 | 5 | 103 | 108 | 1 | 0 | 448 | 462 | 6 | -1 | 190 | 186 | -4 | -2 | 447 | 452 | 0 | 4 | 260 | 260 | 6 | 1 | 221 | 216 | -3 | 0 | 545 | 535 |
| | | | | -3 | -6 | 121 | 121 | 1 | 1 | 286 | 295 | 6 | 0 | 292 | 291 | -4 | 0 | 396 | 385 | 1 | -6 | 50 | 50 | 7 | -2 | 169 | 165 | -3 | 1 | 264 | 265 |
| **** H = 3 **** | | | | -3 | -5 | 160 | 162 | 1 | 2 | 550 | 556 | 6 | 1 | 52 | 51 | -4 | 1 | 203 | 199 | 1 | -5 | 395 | 394 | 7 | -1 | 204 | 199 | -3 | 2 | 317 | 312 |
| -9 | -2 | 95 | 99 | -3 | -4 | 429 | 439 | 1 | 3 | 77 | 74 | 6 | 2 | 256 | 254 | -4 | 2 | 284 | 280 | 1 | -4 | 282 | 283 | | | | | -3 | 3 | 301 | 301 |
| -9 | -1 | 228 | 231 | -3 | -3 | 69 | 65 | 1 | 4 | 358 | 360 | 7 | -4 | 257 | 252 | -4 | 3 | 217 | 221 | 1 | -3 | 242 | 234 | **** H = 5 **** | | | | -3 | 4 | 40 | 35 |
| -9 | 0 | 44 | 35 | -3 | -2 | 608 | 598 | 1 | 5 | 157 | 162 | 7 | -3 | 158 | 149 | -4 | 4 | 92 | 97 | 1 | -2 | 523 | 554 | -9 | -1 | 178 | 183 | -2 | -6 | 200 | 203 |
| -9 | 1 | 275 | 284 | -3 | -1 | 391 | 375 | 2 | -6 | 302 | 303 | 7 | -2 | 200 | 191 | -3 | -6 | 274 | 272 | 1 | -1 | 60 | 63 | -8 | -3 | 175 | 178 | -2 | -5 | 235 | 240 |
| -9 | 2 | 178 | 176 | -3 | 0 | 368 | 349 | 2 | -5 | 78 | 70 | 7 | -1 | 287 | 289 | -3 | -5 | 183 | 179 | 1 | 0 | 541 | 578 | -8 | -2 | 219 | 219 | -2 | -4 | 195 | 200 |
| -8 | -3 | 41 | 39 | -3 | 1 | 645 | 639 | 2 | -4 | 467 | 469 | 7 | 0 | 66 | 63 | -3 | -4 | 273 | 266 | 1 | 1 | 249 | 259 | -8 | -1 | 106 | 103 | -2 | -3 | 300 | 297 |
| -8 | -2 | 366 | 369 | -3 | 2 | 106 | 97 | 2 | -3 | 284 | 292 | 7 | 1 | 272 | 271 | -3 | -3 | 528 | 519 | 1 | 2 | 221 | 224 | -8 | 0 | 286 | 286 | -2 | -1 | 516 | 509 |
| -8 | -1 | 162 | 158 | -3 | 3 | 416 | 420 | 2 | -2 | 339 | 341 | | | | | -3 | -2 | 143 | 143 | 1 | 3 | 406 | 408 | -8 | 2 | 197 | 202 | -2 | 0 | 229 | 223 |
| -8 | 0 | 277 | 280 | -3 | 4 | 197 | 200 | 2 | -1 | 473 | 485 | **** H = 4 **** | | | | -3 | -1 | 596 | 581 | 2 | -6 | 201 | 198 | -7 | -4 | 195 | 209 | -2 | 1 | 313 | 304 |
| -8 | 1 | 294 | 293 | -3 | 5 | 223 | 228 | 2 | 0 | 96 | 97 | -9 | -2 | 180 | 175 | -3 | 0 | 336 | 324 | 2 | -5 | 302 | 303 | -7 | -3 | 259 | 263 | -2 | 2 | 331 | 318 |

Table 6. Observed and calculated structure factors for artroeite.



| K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC | K | L | FO | FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| -2 | 4 | 267 | 260 | 2 | 1 | 215 | 214 | -7 | 1 | 125 | 124 | -2 | -3 | 271 | 275 | 2 | 2 | 165 | 151 | -4 | 1 | 227 | 226 | 2 | -2 | 157 | 161 | | | | |
| -1 | -6 | 165 | 164 | 2 | 2 | 216 | 208 | -6 | -4 | 158 | 167 | -2 | -2 | 360 | 366 | 3 | -5 | 255 | 248 | -4 | 2 | 141 | 138 | 2 | -1 | 210 | 209 | | | | |
| -1 | -5 | 223 | 214 | 2 | 3 | 258 | 254 | -6 | -3 | 218 | 223 | -2 | 0 | 407 | 414 | 3 | -4 | 299 | 287 | -3 | -5 | 240 | 248 | 2 | 0 | 259 | 251 | | | | |
| -1 | -4 | 398 | 405 | 3 | -6 | 222 | 220 | -6 | -2 | 118 | 117 | -2 | 1 | 86 | 89 | 3 | -3 | 77 | 70 | -3 | -3 | 325 | 333 | 3 | -4 | 209 | 203 | | | | |
| -1 | -2 | 516 | 532 | 3 | -5 | 214 | 205 | -6 | -1 | 305 | 306 | -2 | 2 | 238 | 240 | 3 | -2 | 342 | 346 | -3 | -2 | 170 | 171 | 3 | -3 | 201 | 194 | | | | |
| -1 | -1 | 267 | 268 | 3 | -4 | 121 | 120 | -6 | 0 | 63 | 67 | -2 | 3 | 230 | 229 | 3 | -1 | 74 | 75 | -3 | -1 | 239 | 238 | 3 | -2 | 145 | 145 | | | | |
| -1 | 0 | 314 | 322 | 3 | -3 | 450 | 453 | -6 | 1 | 265 | 265 | -1 | -6 | 249 | 260 | 3 | 0 | 230 | 226 | -3 | 0 | 296 | 277 | 3 | -1 | 273 | 272 | | | | |
| -1 | 1 | 444 | 467 | 3 | -2 | 104 | 110 | -6 | 2 | 187 | 188 | -1 | -5 | 179 | 180 | 3 | 1 | 195 | 193 | -3 | 1 | 54 | 50 | | | | | | | | |
| -1 | 3 | 320 | 327 | 3 | -1 | 340 | 343 | -5 | -5 | 261 | 258 | -1 | -4 | 215 | 214 | 4 | -4 | 138 | 132 | -3 | 2 | 257 | 244 | **** H = 8 **** | | | | | | | |
| -1 | 4 | 139 | 138 | 3 | 0 | 330 | 333 | -5 | -4 | 299 | 299 | -1 | -3 | 422 | 425 | 4 | -3 | 252 | 243 | -2 | -4 | 297 | 301 | -6 | -2 | 251 | 248 | | | | |
| 0 | -6 | 122 | 113 | 3 | 1 | 68 | 72 | -5 | -3 | 123 | 127 | -1 | -1 | 401 | 409 | 4 | -1 | 259 | 252 | -2 | -3 | 66 | 67 | -5 | -3 | 227 | 223 | | | | |
| 0 | -5 | 261 | 264 | 3 | 2 | 277 | 280 | -5 | -2 | 398 | 400 | -1 | 0 | 249 | 238 | 4 | 0 | 177 | 174 | -2 | -2 | 268 | 270 | -5 | -2 | 212 | 208 | | | | |
| 0 | -4 | 57 | 57 | 3 | 3 | 47 | 40 | -5 | -1 | 207 | 204 | -1 | 1 | 174 | 183 | 5 | -3 | 101 | 101 | -2 | -1 | 295 | 292 | -5 | -1 | 71 | 57 | | | | |
| 0 | -3 | 434 | 442 | 4 | -5 | 73 | 77 | -5 | 0 | 339 | 329 | -1 | 2 | 285 | 286 | 5 | -2 | 213 | 205 | -2 | 0 | 156 | 155 | -5 | 0 | 253 | 254 | | | | |
| 0 | -2 | 288 | 290 | 4 | -4 | 275 | 273 | -5 | 1 | 270 | 267 | -1 | 3 | 47 | 36 | 5 | -1 | 199 | 198 | -2 | 1 | 374 | 372 | -4 | -4 | 214 | 211 | | | | |
| 0 | -1 | 274 | 281 | 4 | -2 | 265 | 263 | -5 | 2 | 78 | 80 | 0 | -6 | 151 | 148 | | | | | -2 | 2 | 80 | 83 | -4 | -3 | 192 | 197 | | | | |
| 0 | 0 | 410 | 438 | 4 | -1 | 237 | 242 | -5 | 3 | 254 | 260 | 0 | -5 | 173 | 174 | **** H = 7 **** | | | | -1 | -5 | 280 | 276 | -4 | -2 | 166 | 164 | | | | |
| 0 | 1 | 57 | 32 | 4 | 0 | 199 | 196 | -4 | -5 | 192 | 200 | 0 | -4 | 310 | 314 | -7 | -3 | 100 | 102 | -1 | -4 | 221 | 220 | -4 | -1 | 350 | 342 | | | | |
| 0 | 2 | 348 | 352 | 4 | 1 | 283 | 278 | -4 | -4 | 51 | 50 | 0 | -2 | 385 | 392 | -7 | -2 | 246 | 247 | -1 | -3 | 159 | 161 | -4 | 0 | 51 | 46 | | | | |
| 0 | 3 | 123 | 124 | 5 | -4 | 122 | 128 | -4 | -3 | 360 | 366 | 0 | -1 | 149 | 148 | -7 | -1 | 186 | 189 | -1 | -2 | 343 | 344 | -3 | -4 | 232 | 238 | | | | |
| 0 | 4 | 165 | 163 | 5 | -3 | 256 | 256 | -4 | -2 | 149 | 145 | 0 | 0 | 275 | 273 | -7 | 0 | 107 | 111 | -1 | 0 | 269 | 270 | -3 | -2 | 277 | 275 | | | | |
| 1 | -6 | 270 | 270 | 5 | -2 | 331 | 319 | -4 | -1 | 314 | 306 | 0 | 1 | 316 | 318 | -6 | -4 | 54 | 64 | -1 | 1 | 143 | 143 | -3 | -1 | 117 | 110 | | | | |
| 1 | -5 | 54 | 56 | 5 | -1 | 46 | 42 | -4 | 0 | 298 | 300 | 0 | 2 | 88 | 94 | -6 | -3 | 226 | 230 | -1 | 2 | 158 | 167 | -3 | 0 | 185 | 184 | | | | |
| 1 | -4 | 379 | 380 | 5 | 0 | 281 | 283 | -4 | 1 | 70 | 68 | 0 | 3 | 302 | 294 | -6 | -2 | 207 | 218 | 0 | -5 | 85 | 91 | -2 | -4 | 126 | 117 | | | | |
| 1 | -3 | 242 | 240 | 5 | 1 | 108 | 106 | -4 | 2 | 318 | 309 | 1 | -6 | 119 | 118 | -6 | -1 | 115 | 121 | 0 | -4 | 195 | 197 | -2 | -3 | 329 | 327 | | | | |
| 1 | -2 | 204 | 213 | 6 | -3 | 205 | 200 | -4 | 3 | 45 | 38 | 1 | -5 | 359 | 364 | -6 | 0 | 276 | 273 | 0 | -3 | 273 | 269 | -2 | -2 | 78 | 80 | | | | |
| 1 | -1 | 510 | 544 | 6 | -2 | 112 | 111 | -3 | -6 | 236 | 241 | 1 | -4 | 52 | 53 | -5 | -4 | 235 | 233 | 0 | -2 | 113 | 109 | -2 | -1 | 247 | 243 | | | | |
| 1 | 0 | 50 | 34 | 6 | -1 | 247 | 239 | -3 | -5 | 56 | 57 | 1 | -3 | 347 | 353 | -5 | -3 | 240 | 231 | 0 | -1 | 375 | 373 | -2 | 0 | 263 | 264 | | | | |
| 1 | 1 | 365 | 378 | | | | | -3 | -4 | 357 | 359 | 1 | -2 | 315 | 318 | -5 | -2 | 76 | 79 | 0 | 0 | 132 | 132 | -1 | -4 | 233 | 235 | | | | |
| 1 | 2 | 246 | 247 | **** H = 6 **** | | | | -3 | -3 | 229 | 220 | 1 | -1 | 118 | 117 | -5 | -1 | 317 | 320 | 0 | 1 | 230 | 235 | -1 | -3 | 156 | 155 | | | | |
| 1 | 3 | 119 | 110 | -8 | -2 | 184 | 182 | -3 | -2 | 329 | 322 | 1 | 0 | 355 | 363 | -5 | 0 | 92 | 88 | 0 | 2 | 237 | 248 | -1 | -2 | 192 | 197 | | | | |
| 2 | -6 | 50 | 57 | -8 | -1 | 181 | 189 | -3 | -1 | 380 | 372 | 1 | 2 | 211 | 210 | -5 | 1 | 246 | 256 | 1 | -5 | 90 | 91 | -1 | -1 | 260 | 258 | | | | |
| 2 | -5 | 268 | 256 | -8 | 0 | 135 | 144 | -3 | 0 | 62 | 57 | 2 | -4 | 263 | 256 | -4 | -5 | 187 | 193 | 1 | -4 | 313 | 311 | 0 | -4 | 104 | 110 | | | | |
| 2 | -4 | 239 | 249 | -7 | -4 | 78 | 55 | -3 | 1 | 381 | 374 | 2 | -3 | 183 | 180 | -4 | -4 | 232 | 237 | 1 | -2 | 259 | 256 | 0 | -3 | 201 | 198 | | | | |
| 2 | -3 | 181 | 185 | -7 | -3 | 307 | 305 | -3 | 2 | 133 | 129 | 2 | -2 | 226 | 232 | -4 | -3 | 59 | 61 | 1 | -1 | 209 | 208 | 0 | -2 | 272 | 261 | | | | |
| 2 | -2 | 399 | 411 | -7 | -2 | 287 | 286 | -3 | 3 | 206 | 202 | 2 | -1 | 316 | 314 | -4 | -2 | 348 | 338 | 1 | 0 | 179 | 179 | 0 | 0 | 251 | 249 | | | | |
| 2 | -1 | 43 | 27 | -7 | -1 | 153 | 147 | -2 | -5 | 314 | 319 | 2 | 0 | 59 | 53 | -4 | -1 | 57 | 47 | 1 | 1 | 247 | 254 | 1 | -3 | 265 | 258 | | | | |
| 2 | 0 | 354 | 359 | -7 | 0 | 339 | 344 | -2 | -4 | 170 | 173 | 2 | 1 | 316 | 317 | -4 | 0 | 289 | 281 | 2 | -3 | 287 | 274 | 1 | -1 | 218 | 228 | | | | |