

Acta Crystallographica Section C

**Crystal Structure
Communications**

ISSN 0108-2701

Editor: **George Ferguson**

Tris(3-chlorophenyl)phosphine Oxide

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Table 1. Observed and calculated structure factors for 1

| 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 | h | k | l | 10Fo | 10Fc | 10s | |
|----|---|---|------|------|-----|----|-----|---|------|------|-----|----|----|---|------|------|-----|----|----|---|------|------|-----|----|----|---|------|------|-----|---|---|---|------|------|-----|--|
| 1 | 0 | 0 | 197 | 209 | 2 | 3 | 6 | 0 | 64 | 63 | 5 | -1 | -7 | 1 | 170 | 91 | 3 | 3 | -1 | 1 | 338 | 326 | 5 | 3 | 5 | 1 | 42 | 40 | 8 | | | | | | | |
| 2 | 0 | 0 | 131 | 172 | 6 | 4 | 6 | 0 | 48 | 47 | 8 | 0 | -7 | 1 | 98 | 169 | 3 | 4 | -1 | 1 | 29 | 36 | 6 | 4 | 5 | 1 | 50 | 52 | 7 | | | | | | | |
| 3 | 0 | 0 | 232 | 219 | 5 | 5 | 6 | 0 | 13 | 15 | 12 | 0 | -7 | 1 | 125 | 122 | 2 | 5 | -1 | 1 | 65 | 55 | 3 | 5 | 5 | 1 | 40 | 24 | 9 | | | | | | | |
| 4 | 0 | 0 | 17 | 9 | 17 | -7 | 7 | 0 | 24 | 31 | 24 | 2 | -7 | 1 | 21 | 0 | 20 | 6 | -1 | 1 | 29 | 27 | 11 | 6 | 5 | 1 | 30 | 8 | 20 | | | | | | | |
| 5 | 0 | 0 | 50 | 60 | 6 | -6 | 7 | 0 | 28 | 28 | 18 | 3 | -7 | 1 | 136 | 143 | 4 | 7 | -1 | 1 | 25 | 23 | 20 | -7 | 6 | 1 | 48 | 36 | 7 | | | | | | | |
| 6 | 0 | 0 | 65 | 74 | 6 | -5 | 7 | 0 | 0 | 16 | 1 | 4 | -7 | 1 | 41 | 42 | 9 | -7 | 0 | 1 | 43 | 44 | 9 | -6 | 6 | 1 | 26 | 27 | 21 | | | | | | | |
| 7 | 0 | 0 | 0 | 0 | 2 | -4 | 7 | 0 | 17 | 7 | 17 | 5 | -7 | 1 | 74 | 76 | 4 | -6 | 0 | 1 | 0 | 9 | 1 | -5 | 6 | 1 | 97 | 102 | 3 | | | | | | | |
| -7 | 1 | 0 | 3 | 2 | 2 | -3 | 7 | 0 | 206 | 206 | 5 | 6 | -7 | 1 | 13 | 24 | 12 | -5 | 0 | 1 | 23 | 39 | 22 | -4 | 6 | 1 | 51 | 46 | 6 | | | | | | | |
| -6 | 1 | 0 | 31 | 28 | 10 | -2 | 7 | 0 | 20 | 15 | 20 | 7 | -7 | 1 | 25 | 22 | 24 | -4 | 0 | 1 | 129 | 125 | 2 | -3 | 6 | 1 | 216 | 214 | 5 | | | | | | | |
| -5 | 1 | 0 | 153 | 145 | 3 | -1 | 7 | 0 | 241 | 242 | 4 | -5 | -6 | 1 | 88 | 79 | 5 | -3 | 0 | 1 | 504 | 504 | 5 | -2 | 6 | 1 | 234 | 223 | 5 | | | | | | | |
| -4 | 1 | 0 | 197 | 211 | 5 | 0 | 7 | 0 | 161 | 156 | 2 | -4 | -6 | 1 | 53 | 49 | 7 | -2 | 0 | 1 | 68 | 85 | 2 | -1 | 6 | 1 | 52 | 40 | 5 | | | | | | | |
| -3 | 1 | 0 | 26 | 39 | 7 | 1 | 7 | 0 | 192 | 191 | 4 | -3 | -6 | 1 | 89 | 98 | 4 | -1 | 0 | 1 | 641 | 648 | 2 | 0 | 6 | 1 | 32 | 36 | 10 | | | | | | | |
| -2 | 1 | 0 | 130 | 140 | 3 | 2 | 7 | 0 | 0 | 9 | 1 | -2 | -6 | 1 | 113 | 112 | 4 | 1 | 0 | 1 | 266 | 268 | 1 | 1 | 6 | 1 | 98 | 93 | 2 | | | | | | | |
| -1 | 1 | 0 | 61 | 60 | 4 | 3 | 7 | 0 | 37 | 34 | 11 | -1 | -6 | 1 | 248 | 253 | 5 | 2 | 0 | 1 | 291 | 303 | 4 | 2 | 6 | 1 | 103 | 112 | 4 | | | | | | | |
| 0 | 1 | 0 | 248 | 210 | 4 | 4 | 7 | 0 | 0 | 18 | 1 | 0 | -6 | 1 | 15 | 15 | 15 | 3 | 0 | 1 | 14 | 27 | 14 | 3 | 6 | 1 | 12 | 26 | 11 | | | | | | | |
| 1 | 1 | 0 | 433 | 426 | 2 | 5 | 7 | 0 | 0 | 12 | 1 | 1 | -6 | 1 | 207 | 196 | 3 | 4 | 0 | 1 | 105 | 105 | 2 | 5 | 6 | 1 | 37 | 31 | 11 | | | | | | | |
| 2 | 1 | 0 | 274 | 266 | 4 | -6 | 8 | 0 | 29 | 27 | 19 | 2 | -6 | 1 | 141 | 130 | 3 | 5 | 0 | 1 | 45 | 56 | 6 | -5 | 6 | 1 | 10 | 5 | 10 | | | | | | | |
| 3 | 1 | 0 | 132 | 155 | 6 | -5 | 8 | 0 | 79 | 87 | 4 | 3 | -6 | 1 | 57 | 52 | 5 | 6 | 0 | 1 | 20 | 22 | 19 | -7 | 7 | 1 | 54 | 53 | 7 | | | | | | | |
| 4 | 1 | 0 | 48 | 65 | 5 | -4 | 8 | 0 | 37 | 34 | 10 | 4 | -6 | 1 | 69 | 64 | 5 | 7 | 0 | 1 | 0 | 3 | 1 | -6 | 7 | 1 | 79 | 86 | 5 | | | | | | | |
| 5 | 1 | 0 | 181 | 166 | 5 | -3 | 8 | 0 | 75 | 70 | 4 | 5 | -6 | 1 | 19 | 11 | 18 | -7 | 1 | 1 | 47 | 43 | 6 | -5 | 7 | 1 | 40 | 26 | 9 | | | | | | | |
| 6 | 1 | 0 | 0 | 30 | 1 | -2 | 8 | 0 | 59 | 53 | 6 | 6 | -6 | 1 | 48 | 53 | 7 | -6 | 1 | 1 | 62 | 64 | 4 | -4 | 7 | 1 | 181 | 183 | 4 | | | | | | | |
| 7 | 1 | 0 | 15 | 9 | 15 | -1 | 8 | 0 | 51 | 62 | 5 | 7 | -6 | 1 | 29 | 25 | 18 | -5 | 1 | 1 | 15 | 0 | 14 | -3 | 7 | 1 | 30 | 18 | 13 | | | | | | | |
| -6 | 2 | 0 | 0 | 5 | 1 | 1 | 1 | 8 | 66 | 70 | 3 | -5 | -5 | 1 | 47 | 55 | 8 | -4 | 1 | 1 | 120 | 108 | 3 | -2 | 7 | 1 | 61 | 63 | 5 | | | | | | | |
| -5 | 2 | 0 | 136 | 127 | 3 | 2 | 8 | 0 | 78 | 83 | 5 | -4 | -5 | 1 | 25 | 33 | 25 | -2 | 1 | 1 | 529 | 560 | 2 | -1 | 7 | 1 | 148 | 143 | 3 | | | | | | | |
| -4 | 2 | 0 | 131 | 121 | 3 | 3 | 8 | 0 | 23 | 28 | 23 | -3 | -5 | 1 | 123 | 97 | 3 | -1 | 1 | 1 | 656 | 679 | 6 | 0 | 7 | 1 | 143 | 134 | 6 | | | | | | | |
| -3 | 2 | 0 | 244 | 232 | 6 | 4 | 8 | 0 | 44 | 45 | 11 | -2 | -5 | 1 | 14 | 21 | 14 | 0 | 1 | 1 | 36 | 39 | 2 | 2 | 7 | 1 | 57 | 60 | 6 | | | | | | | |
| -2 | 2 | 0 | 218 | 212 | 5 | -6 | 9 | 0 | 17 | 6 | 16 | -1 | -5 | 1 | 0 | 8 | 1 | -1 | 1 | 1 | 86 | 91 | 5 | 3 | 7 | 1 | 75 | 62 | 5 | | | | | | | |
| -1 | 2 | 0 | 493 | 437 | 8 | -5 | 9 | 0 | 61 | 59 | 6 | 0 | 0 | 1 | 79 | 70 | 2 | 2 | 1 | 1 | 458 | 474 | 4 | 4 | 7 | 1 | 5 | 9 | 5 | | | | | | | |
| 0 | 2 | 0 | 401 | 355 | 2 | -4 | 9 | 0 | 0 | 3 | 1 | 1 | -5 | 1 | 65 | 69 | 2 | 3 | 1 | 1 | 51 | 71 | 4 | 5 | 7 | 1 | 0 | 2 | 1 | | | | | | | |
| 1 | 2 | 0 | 402 | 372 | 2 | -3 | 9 | 0 | 15 | 6 | 15 | 2 | -5 | 1 | 34 | 36 | 7 | 4 | 1 | 1 | 30 | 31 | 9 | -6 | 8 | 1 | 40 | 43 | 10 | | | | | | | |
| 2 | 2 | 0 | 239 | 236 | 5 | -2 | 9 | 0 | 30 | 37 | 15 | 3 | -5 | 1 | 317 | 309 | 6 | 5 | 1 | 1 | 116 | 138 | 5 | -5 | 8 | 1 | 27 | 27 | 17 | | | | | | | |
| 3 | 2 | 0 | 79 | 101 | 4 | -1 | 9 | 0 | 134 | 128 | 2 | 4 | -5 | 1 | 284 | 287 | 7 | 6 | 1 | 1 | 48 | 56 | 7 | -4 | 8 | 1 | 150 | 163 | 3 | | | | | | | |
| 4 | 2 | 0 | 159 | 147 | 3 | 0 | 9 | 0 | 104 | 99 | 2 | 5 | -5 | 1 | 23 | 16 | 22 | 7 | 1 | 1 | 38 | 41 | 12 | -3 | 8 | 1 | 48 | 50 | 7 | | | | | | | |
| 5 | 2 | 0 | 73 | 83 | 5 | 1 | 9 | 0 | 40 | 41 | 7 | 6 | -5 | 1 | 63 | 73 | 5 | -8 | 2 | 1 | 39 | 27 | 12 | -2 | 8 | 1 | 58 | 59 | 6 | | | | | | | |
| 6 | 2 | 0 | 51 | 48 | 7 | 2 | 9 | 0 | 24 | 31 | 24 | 7 | -5 | 1 | 0 | 11 | 1 | -7 | 2 | 1 | 27 | 16 | 12 | -1 | 8 | 1 | 160 | 162 | 2 | | | | | | | |
| 7 | 2 | 0 | 29 | 20 | 20 | 3 | 9 | 0 | 25 | 9 | 24 | -6 | -4 | 1 | 17 | 4 | 17 | -6 | 2 | 1 | 36 | 42 | 17 | 0 | 8 | 1 | 23 | 18 | 16 | | | | | | | |
| -7 | 3 | 0 | 15 | 22 | 14 | -5 | 10 | 0 | 41 | 46 | 10 | -5 | -4 | 1 | 29 | 40 | 15 | -5 | 2 | 1 | 16 | 14 | 15 | -5 | 2 | 1 | 53 | 56 | 4 | | | | | | | |
| -6 | 3 | 0 | 24 | 35 | 23 | -4 | 10 | 0 | 0 | 1 | 1 | -4 | -4 | 1 | 60 | 67 | 5 | -4 | 2 | 1 | 62 | 58 | 13 | 1 | 8 | 1 | 5 | 14 | 4 | | | | | | | |
| -5 | 3 | 0 | 20 | 3 | 20 | -3 | 10 | 0 | 75 | 84 | 5 | -3 | -4 | 1 | 70 | 83 | 4 | -3 | 2 | 1 | 335 | 319 | 5 | 3 | 8 | 1 | 3 | 9 | 9 | | | | | | | |
| -4 | 3 | 0 | 27 | 24 | 10 | -2 | 10 | 0 | 78 | 82 | 5 | -2 | -4 | 1 | 162 | 149 | 3 | -2 | 2 | 1 | 339 | 330 | 4 | 4 | 8 | 1 | 38 | 39 | 13 | | | | | | | |
| -3 | 3 | 0 | 241 | 232 | 5 | -1 | 10 | 0 | 25 | 30 | 19 | -1 | -4 | 1 | 97 | 102 | 5 | -1 | 1 | 1 | 664 | 616 | 2 | -6 | 9 | 1 | 46 | 50 | 9 | | | | | | | |
| -2 | 3 | 0 | 350 | 332 | 4 | 0 | 10 | 0 | 0 | 9 | 1 | 0 | -4 | 1 | 264 | 232 | 4 | 0 | 2 | 1 | 902 | 815 | 6 | -5 | 9 | 1 | 27 | 26 | 22 | | | | | | | |
| -1 | 3 | 0 | 80 | 65 | 4 | 1 | 10 | 0 | 72 | 65 | 4 | 1 | -4 | 1 | 375 | 346 | 3 | 1 | 2 | 1 | 409 | 410 | 7 | -4 | 9 | 1 | 134 | 135 | 3 | | | | | | | |
| 0 | 3 | 0 | 79 | 78 | 2 | 2 | 10 | 0 | 0 | 9 | 1 | 2 | -4 | 1 | 252 | 223 | 5 | 2 | 2 | 1 | 187 | 179 | 4 | -3 | 9 | 1 | 0 | 27 | 1 | | | | | | | |
| 1 | 3 | 0 | 172 | 182 | 6 | -4 | 11 | 0 | 26 | 14 | 25 | 3 | -4 | 1 | 295 | 278 | 6 | 3 | 2 | 1 | 353 | 338 | 6 | -2 | 9 | 1 | 0 | 8 | 1 | | | | | | | |
| 2 | 3 | 0 | 294 | 264 | 1 | -3 | 11 | 0 | 0 | 5 | 1 | 4 | -4 | 1 | 75 | 71 | 4 | 4 | 2 | 1 | 63 | 76 | 5 | -1 | 9 | 1 | 26 | 28 | 12 | | | | | | | |
| 3 | 3 | 0 | 77 | 107 | 3 | -2 | 11 | 0 | 20 | 15 | 19 | 5 | -4 | 1 | 123 | 126 | 4 | 5 | 2 | 1 | 17 | 10 | 16 | 0 | 9 | 1 | 75 | 78 | 3 | | | | | | | |
| 4 | 3 | 0 | 169 | 159 | 3 | 0 | 11 | 0 | 49 | 54 | 6 | 6 | -4 | 1 | 0 | 12 | 1 | 6 | 2 | 1 | 15 | 14 | 14 | 1 | 9 | 1 | 48 | 47 | 5 | | | | | | | |
| 5 | 3 | 0 | 30 | 36 | 13 | -1 | 11 | 0 | 54 | 52 | 5 | 7 | -4 | 1 | 48 | 46 | 8 | 7 | 3 | 1 | 11 | 15 | 11 | 2 | 9 | 1 | 59 | 56 | 7 | | | | | | | |
| 6 | 3 | 0 | 37 | 27 | 11 | 1 | 11 | 0 | 24 | 21 | 23 | -7 | -3 | 1 | 38 | 34 | 14 | -8 | 3 | 1 | 32 | 28 | 14 | -5 | 10 | 1 | 18 | 23 | 18 | | | | | | | |
| 7 | 3 | 0 | 20 | 13 | 20 | -1 | -11 | 1 | 14 | 8 | 14 | -6 | -3 | 1 | 6 | 23 | 6 | -7 | 3 | 1 | 19 | 13 | 19 | -5 | 10 | 1 | 35 | 30 | 12 | | | | | | | |
| -6 | 4 | 0 | 40 | 35 | 10 | 0 | -11 | 1 | 10 | 11 | 9 | -5 | -3 | 1 | 21 | 40 | 20 | -6 | 3 | 1 | 116 | 110 | 3 | -4 | 10 | 1 | 35 | 30 | 12 | | | | | | | |
| -5 | 4 | 0 | 30 | 40 | 13 | 1 | -11 | 1 | 44 | 40 | 6 | -4 | -3 | 1 | 49 | 53 | 6 | -5 | 3 | 1 | 50 | 57 | 5 | -3 | 10 | 1 | 10 | 11 | 10 | | | | | | | |
| -4 | 4 | 0 | 86 | 90 | 3 | 2 | -11 | 1 | 60 | 58 | 7 | -3 | -3 | 1 | 21 | 33 | 21 | -4 | 3 | 1 | 132 | 128 | 3 | -2 | 10 | | | | | | | | | | | |

Table 1. Observed and calculated structure factors for 1.

| Observed | | | Calculated | | | Observed | | | Calculated | | | | | | | | |
|----------|------|----|------------|------|-----|----------|----|----|------------|------|-----|----|----|-----|------|------|-----|
| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
| 90 | 93 | 4 | 231 | 250 | 7 | 2 | 4 | 2 | 239 | 221 | 5 | 2 | 4 | 2 | 239 | 221 | 5 |
| 13 | 15 | 13 | 23 | 29 | 22 | 2 | 4 | 2 | 55 | 70 | 5 | 3 | 10 | 3 | 111 | 109 | 4 |
| 86 | 82 | 3 | 34 | 36 | 9 | 4 | 4 | 4 | 96 | 111 | 4 | 5 | 10 | 78 | 83 | 5 | |
| 76 | 69 | 3 | 7 | 17 | 6 | 4 | 4 | 4 | 64 | 61 | 6 | 5 | 10 | 28 | 31 | 27 | |
| 55 | 54 | 4 | 21 | 4 | 21 | 5 | 6 | 4 | 0 | 2 | 1 | -3 | -9 | 15 | 28 | 14 | |
| 174 | 179 | 4 | 99 | 108 | 5 | -7 | 5 | 5 | 0 | 0 | 1 | -2 | -9 | 0 | 0 | 1 | |
| 150 | 150 | 4 | 143 | 130 | 3 | -5 | 5 | 5 | 10 | 23 | 10 | -1 | -9 | 18 | 24 | 18 | |
| 38 | 44 | 10 | 187 | 228 | 7 | -5 | 5 | 5 | 23 | 2 | 23 | 0 | -9 | 43 | 46 | 6 | |
| 49 | 61 | 8 | 210 | 198 | 5 | -4 | 4 | 4 | 168 | 183 | 6 | 1 | -9 | 48 | 47 | 6 | |
| 10 | 6 | 10 | 154 | 197 | 6 | -3 | 3 | 3 | 365 | 369 | 6 | 2 | -9 | 115 | 111 | 3 | |
| 37 | 36 | 13 | 539 | 543 | 2 | -2 | 2 | 2 | 268 | 283 | 6 | 4 | -9 | 66 | 70 | 6 | |
| 0 | 0 | 1 | 260 | 250 | 2 | -1 | 1 | 1 | 90 | 85 | 2 | 5 | -9 | 48 | 48 | 8 | |
| 54 | 54 | 7 | 456 | 450 | 3 | 0 | 0 | 0 | 39 | 38 | 4 | 6 | -9 | 11 | 3 | 23 | |
| 154 | 130 | 2 | 201 | 194 | 4 | 1 | 1 | 1 | 32 | 31 | 6 | 6 | -9 | 24 | 8 | 8 | |
| 127 | 122 | 3 | 192 | 199 | 4 | 4 | 4 | 4 | 121 | 101 | 2 | -4 | -8 | 46 | 32 | 10 | |
| 207 | 195 | 3 | 13 | 11 | 12 | 3 | 3 | 3 | 110 | 116 | 4 | -3 | -8 | 35 | 26 | 13 | |
| 158 | 151 | 4 | 27 | 18 | 10 | 4 | 4 | 4 | 103 | 107 | 4 | -2 | -8 | 32 | 36 | 14 | |
| 19 | 17 | 19 | 20 | 23 | 20 | 5 | 5 | 5 | 19 | 1 | 19 | -1 | -8 | 89 | 90 | 3 | |
| 86 | 88 | 4 | 25 | 3 | 18 | 6 | 6 | 6 | 17 | 15 | 17 | 0 | -8 | 204 | 190 | 5 | |
| 34 | 34 | 11 | 9 | 14 | 8 | -7 | 7 | 7 | 28 | 23 | 17 | 1 | -8 | 26 | 24 | 11 | |
| 43 | 40 | 9 | 68 | 75 | 4 | -6 | 6 | 6 | 34 | 27 | 10 | 2 | -8 | 8 | 21 | 7 | |
| 34 | 31 | 12 | 32 | 45 | 9 | -5 | 5 | 5 | 44 | 46 | 7 | 3 | -8 | 98 | 94 | 4 | |
| 41 | 38 | 11 | 44 | 52 | 4 | -4 | 4 | 4 | 168 | 170 | 4 | 4 | -8 | 16 | 2 | 16 | |
| 47 | 43 | 9 | 46 | 37 | 3 | -3 | 3 | 3 | 71 | 75 | 2 | 5 | -8 | 30 | 9 | 14 | |
| 46 | 50 | 8 | 193 | 189 | 4 | -2 | 2 | 2 | 115 | 117 | 4 | 6 | -8 | 30 | 30 | 17 | |
| 0 | 2 | 1 | 213 | 200 | 2 | -1 | 1 | 1 | 104 | 103 | 2 | -5 | -7 | 43 | 40 | 11 | |
| 207 | 194 | 4 | 276 | 280 | 2 | 0 | 0 | 0 | 64 | 61 | 3 | -4 | -7 | 15 | 10 | 14 | |
| 191 | 189 | 4 | 434 | 438 | 2 | 1 | 1 | 1 | 28 | 23 | 3 | -3 | -7 | 41 | 26 | 9 | |
| 100 | 91 | 2 | 121 | 120 | 2 | 2 | 2 | 2 | 165 | 157 | 2 | -2 | -7 | 55 | 45 | 6 | |
| 53 | 51 | 3 | 144 | 141 | 3 | 3 | 3 | 3 | 43 | 39 | 2 | -1 | -7 | 32 | 27 | 8 | |
| 66 | 57 | 4 | 173 | 157 | 3 | 4 | 4 | 4 | 24 | 33 | 24 | 0 | -7 | 73 | 68 | 3 | |
| 11 | 25 | 11 | 129 | 114 | 3 | 5 | 5 | 5 | 0 | 8 | 8 | 1 | -7 | 125 | 123 | 3 | |
| 121 | 119 | 3 | 0 | 17 | 1 | 7 | 7 | 7 | 77 | 75 | 5 | 2 | -7 | 95 | 103 | 3 | |
| 46 | 47 | 7 | 0 | 0 | 3 | -6 | 6 | 6 | 61 | 67 | 5 | 4 | -7 | 102 | 107 | 3 | |
| 36 | 24 | 11 | 0 | 12 | 1 | -5 | 5 | 5 | 69 | 73 | 5 | 5 | -7 | 75 | 81 | 4 | |
| 51 | 52 | 8 | 73 | 70 | 3 | -4 | 4 | 4 | 29 | 20 | 14 | 6 | -7 | 111 | 116 | 3 | |
| 48 | 47 | 10 | 113 | 114 | 3 | -3 | 3 | 3 | 73 | 75 | 4 | 4 | -7 | 0 | 9 | 12 | |
| 0 | 2 | 1 | 191 | 189 | 4 | -2 | 2 | 2 | 73 | 75 | 3 | -5 | -6 | 39 | 24 | 12 | |
| 65 | 79 | 6 | 123 | 108 | 3 | -1 | 1 | 1 | 63 | 55 | 3 | -4 | -6 | 47 | 38 | 9 | |
| 51 | 51 | 6 | 440 | 454 | 3 | 0 | 0 | 0 | 187 | 181 | 3 | -4 | -6 | 39 | 37 | 10 | |
| 91 | 92 | 4 | 763 | 773 | 3 | 1 | 1 | 1 | 75 | 69 | 3 | -3 | -6 | 18 | 1 | 18 | |
| 130 | 122 | 7 | 115 | 104 | 3 | 2 | 2 | 2 | 13 | 20 | 13 | -2 | -6 | 54 | 64 | 6 | |
| 539 | 502 | 4 | 247 | 235 | 4 | 3 | 3 | 3 | 0 | 11 | 11 | -1 | -6 | 247 | 237 | 4 | |
| 166 | 158 | 2 | 172 | 183 | 4 | 4 | 4 | 4 | 25 | 38 | 24 | 0 | -6 | 326 | 306 | 5 | |
| 17 | 16 | 16 | 112 | 137 | 4 | 5 | 5 | 5 | 12 | 5 | 11 | 1 | -6 | 34 | 32 | 6 | |
| 220 | 229 | 6 | 151 | 184 | 4 | 6 | 6 | 6 | 33 | 12 | 13 | 2 | -6 | 60 | 55 | 5 | |
| 32 | 30 | 11 | 85 | 98 | 4 | -5 | 5 | 5 | 133 | 139 | 3 | 2 | -6 | 118 | 118 | 3 | |
| 94 | 99 | 3 | 33 | 30 | 11 | -4 | 4 | 4 | 72 | 74 | 5 | 4 | -6 | 39 | 37 | 9 | |
| 63 | 54 | 5 | 24 | 27 | 23 | -3 | 3 | 3 | 80 | 85 | 4 | 5 | -6 | 77 | 86 | 4 | |
| 17 | 27 | 17 | 20 | 15 | 19 | -2 | 2 | 2 | 6 | 0 | 11 | 1 | -6 | 42 | 47 | 9 | |
| 38 | 21 | 11 | 60 | 51 | 4 | -1 | 1 | 1 | 11 | 5 | 11 | 6 | -6 | 20 | 9 | 20 | |
| 6 | 5 | 5 | 61 | 49 | 4 | 0 | 0 | 0 | 11 | 5 | 11 | 5 | -6 | 0 | 6 | 1 | |
| 113 | 129 | 4 | 39 | 32 | 6 | -5 | 5 | 5 | 100 | 95 | 2 | -4 | -5 | 41 | 44 | 9 | |
| 21 | 21 | 20 | 110 | 103 | 3 | -4 | 4 | 4 | 21 | 13 | 20 | -4 | -5 | 14 | 13 | 14 | |
| 173 | 201 | 6 | 70 | 88 | 2 | -3 | 3 | 3 | 0 | 0 | 2 | -2 | -5 | 200 | 237 | 8 | |
| 44 | 45 | 3 | 19 | 3 | 11 | -4 | 4 | 4 | 23 | 14 | 23 | -3 | -5 | 12 | 21 | 12 | |
| 22 | 9 | 21 | 499 | 478 | 2 | -6 | 6 | 6 | 0 | 17 | 1 | -1 | -5 | 64 | 61 | 3 | |
| 29 | 12 | 5 | 1062 | 990 | 2 | -5 | 5 | 5 | 56 | 61 | 7 | 0 | -5 | 178 | 164 | 2 | |
| 242 | 225 | 10 | 211 | 208 | 6 | -4 | 4 | 4 | 56 | 52 | 7 | 1 | -5 | 0 | 7 | 1 | |
| 27 | 22 | 10 | 31 | 42 | 6 | -3 | 3 | 3 | 62 | 57 | 6 | 2 | -5 | 213 | 199 | 5 | |
| 64 | 72 | 4 | 82 | 108 | 3 | -2 | 2 | 2 | 31 | 37 | 14 | 3 | -5 | 119 | 116 | 3 | |
| 230 | 225 | 5 | 29 | 27 | 11 | -1 | 1 | 1 | 38 | 35 | 7 | 4 | -5 | 177 | 172 | 4 | |
| 39 | 47 | 9 | 0 | 0 | 9 | 0 | 0 | 0 | 88 | 88 | 3 | 5 | -5 | 26 | 15 | 18 | |
| 0 | 0 | 1 | 18 | 14 | 18 | -1 | 1 | 1 | 36 | 35 | 8 | 6 | -5 | 82 | 89 | 4 | |
| 0 | 0 | 3 | 20 | 21 | 20 | 0 | 0 | 0 | 32 | 26 | 16 | 7 | -5 | 27 | 20 | 15 | |
| 62 | 59 | 7 | 33 | 23 | 15 | -6 | 6 | 6 | 51 | 62 | 9 | 5 | -4 | 66 | 68 | 5 | |
| 130 | 116 | 2 | 17 | 21 | 17 | -4 | 4 | 4 | 17 | 21 | 17 | -4 | -4 | 35 | 44 | 10 | |
| 39 | 45 | 6 | 136 | 137 | 10 | -3 | 3 | 3 | 39 | 33 | 10 | -2 | -4 | 69 | 76 | 4 | |
| 239 | 221 | 5 | 89 | 86 | 2 | -2 | 2 | 2 | 100 | 100 | 4 | -3 | -4 | 257 | 246 | 6 | |
| 2 | 10 | 2 | 144 | 136 | 3 | -1 | 1 | 1 | 38 | 41 | 7 | 0 | -4 | 92 | 98 | 2 | |
| 129 | 116 | 3 | 86 | 81 | 6 | 0 | 0 | 0 | 46 | 44 | 6 | -1 | -4 | 73 | 69 | 2 | |
| 235 | 218 | 3 | 360 | 330 | 5 | -1 | 1 | 1 | 106 | 105 | 3 | 1 | -4 | 184 | 171 | 6 | |
| 169 | 162 | 4 | 245 | 231 | 2 | -2 | 2 | 2 | 33 | 36 | 16 | -4 | -4 | 541 | 532 | 5 | |
| 14 | 15 | 13 | 114 | 113 | 2 | -4 | 4 | 4 | 5 | 6 | 5 | 3 | -4 | 73 | 74 | 3 | |
| 68 | 73 | 4 | 157 | 191 | 6 | -3 | 3 | 3 | 15 | 14 | 15 | 4 | -4 | 54 | 59 | 5 | |
| 163 | 156 | 3 | 65 | 81 | 4 | -2 | 2 | 2 | 22 | 10 | 22 | 4 | -4 | 0 | 5 | 5 | |
| 71 | 78 | 4 | 95 | 112 | 4 | -1 | 1 | 1 | 99 | 100 | 3 | 6 | -4 | 70 | 66 | 5 | |
| 52 | 39 | 7 | 29 | 26 | 14 | 0 | 0 | 0 | 63 | 58 | 5 | 7 | -4 | 68 | 56 | 17 | |
| 18 | 17 | 18 | 0 | 0 | 1 | 1 | 1 | 1 | 38 | 39 | 9 | -7 | -3 | 17 | 14 | 17 | |
| 25 | 12 | 24 | 0 | 0 | 3 | -1 | 1 | 1 | 39 | 43 | 9 | -6 | -3 | 0 | 18 | 19 | |
| 0 | 4 | 4 | 0 | 0 | 15 | 0 | 0 | 0 | 48 | 52 | 6 | -5 | -3 | 0 | 23 | 7 | |
| 66 | 78 | 4 | 0 | 0 | 7 | -2 | 2 | 2 | 82 | 85 | 5 | -3 | -3 | 37 | 55 | 2 | |
| 49 | 58 | 5 | 252 | 261 | 3 | -4 | 4 | 4 | 26 | 17 | 26 | -2 | -3 | 104 | 115 | 2 | |
| 335 | 347 | 2 | 138 | 138 | 7 | -4 | 4 | 4 | 50 | 56 | 6 | -5 | -3 | 128 | 113 | 2 | |
| 661 | 639 | 3 | 208 | 181 | 4 | -2 | 2 | 2 | 22 | 10 | 21 | 0 | -3 | 21 | 6 | 8 | |
| 1187 | 1072 | 4 | 648 | 605 | 3 | -1 | 1 | 1 | 46 | 45 | 4 | -1 | -3 | 0 | 4 | 4 | |
| 627 | 588 | 3 | 301 | 291 | 3 | 0 | 0 | 0 | 107 | 101 | 2 | 0 | -3 | 66 | 69 | 3 | |
| 132 | 124 | 3 | 61 | 56 | 2 | -1 | 1 | 1 | 50 | 53 | 5 | 0 | -3 | 322 | 319 | 6 | |
| 450 | 435 | 5 | 291 | 288 | 6 | 4 | 4 | 4 | 291 | 288 | 6 | 4 | -3 | 291 | 288 | 6 | |
| | | | 62 | 69 | 5 | 5 | 5 | 5 | 62 | 69 | 5 | 5 | -3 | 62 | 69 | 5 | |
| | | | 0 | 3 | 1 | 6 | 6 | 6 | 0 | 3 | 1 | 6 | -3 | 0 | 3 | 1 | |
| | | | 20 | 16 | 20 | 7 | 7 | 7 | 20 | 16 | 20 | 7 | -3 | 20 | 16 | 20 | |
| | | | 26 | 24 | 26 | 8 | 8 | 8 | 26 | 24 | 26 | 8 | -3 | 26 | 24 | 26 | |
| | | | 44 | 44 | 44 | 9 | 9 | 9 | 44 | 44 | 44 | 9 | -3 | 44 | 44 | 44 | |
| | | | 66 | 65 | 66 | 10 | 10 | 10 | 66 | 65 | 66 | 10 | -3 | 66 | 65 | 66 | |
| | | | 35 | 40 | 35 | 11 | 11 | 11 | 35 | 40 | 35 | 11 | -3 | 35 | 40 | 35 | |
| | | | 392 | 354 | 392 | 12 | 12 | 12 | 392 | 354 | 392 | 12 | -3 | 392 | 354 | 392 | |
| | | | 20 | 20 | 20 | 13 | 13 | 13 | 20 | 20 | 20 | 13 | -3 | 20 | 20 | 20 | |
| | | | 625 | 590 | 625 | 14 | 14 | 14 | 625 | 590 | 625 | 14 | -3 | 625 | 590 | 625 | |
| | | | 690 | 636 | 690 | 15 | 15 | 15 | 690 | 636 | 690 | 15 | -3 | 690 | 636 | 690 | |
| | | | 192 | 174 | 192 | 16 | 16 | 16 | 192 | 174 | 192 | 16 | -3 | 192 | 174 | 192 | |
| | | | 320 | 308 | 320 | 17 | 17 | 17 | 320 | 308 | 320 | 17 | -3 | 320 | 308 | 320 | |
| | | | 63 | 66 | 63 | 18 | 18 | 18 | 63 | 66 | 63 | | | | | | |

Table 1. Observed and calculated structure factors for 1.

| | | | Observed | | | | | | | | | Calculated | | | | | | | | | | | | | | |
|----|----|---|----------|------|-----|---|---|---|------|------|-----|------------|-----|------|------|------|-----|-----|-----|----|------|------|-----|-----|-----|----|
| 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 | -4 | 5 | 134 | 126 | 3 | 2 | 2 | 5 | 33 | 35 | 6 | 13 | 23 | 12 | 1 | -4 | 6 | 25 | 18 | 7 | 1 | 2 | 6 | 107 | 109 | 1 |
| 3 | -4 | 5 | 63 | 70 | 4 | 2 | 2 | 5 | 100 | 112 | 5 | 13 | 9 | 13 | 2 | -4 | 6 | 132 | 140 | 3 | 2 | 2 | 6 | 186 | 211 | 6 |
| 4 | -4 | 5 | 97 | 103 | 3 | 2 | 2 | 5 | 106 | 127 | 5 | 23 | 1 | 22 | 3 | -4 | 6 | 212 | 207 | 5 | 3 | 2 | 6 | 122 | 132 | 4 |
| 5 | -4 | 5 | 35 | 34 | 3 | 2 | 2 | 5 | 61 | 64 | 1 | 42 | 41 | 10 | 4 | -4 | 6 | 40 | 41 | 8 | 4 | 2 | 6 | 82 | 96 | 4 |
| 6 | -4 | 5 | 27 | 28 | 13 | 2 | 2 | 5 | 1 | 1 | 1 | 59 | 47 | 6 | 5 | -4 | 6 | 0 | 10 | 1 | 5 | 2 | 6 | 88 | 89 | 3 |
| 7 | -4 | 5 | 35 | 34 | 10 | 2 | 2 | 5 | 70 | 60 | 4 | 62 | 60 | 6 | 6 | -4 | 6 | 17 | 5 | 16 | 6 | 2 | 6 | 25 | 15 | 24 |
| 8 | -4 | 5 | 37 | 30 | 11 | 2 | 2 | 5 | 67 | 57 | 4 | 54 | 52 | 5 | 7 | -4 | 6 | 0 | 7 | 7 | 7 | 3 | 6 | 19 | 25 | 18 |
| 9 | -4 | 5 | 18 | 30 | 17 | 2 | 2 | 5 | 136 | 126 | 3 | 25 | 24 | 15 | -7 | -3 | 6 | 38 | 25 | 12 | -6 | 3 | 6 | 52 | 53 | 5 |
| 10 | -4 | 5 | 37 | 31 | 11 | 2 | 2 | 5 | 174 | 174 | 3 | 18 | 15 | 18 | -6 | -3 | 6 | 41 | 35 | 9 | -5 | 3 | 6 | 192 | 199 | 4 |
| 11 | -4 | 5 | 10 | 9 | 9 | 2 | 2 | 5 | 7 | 16 | 6 | 18 | 13 | 17 | -5 | -3 | 6 | 12 | 9 | 11 | -4 | 3 | 6 | 42 | 40 | 5 |
| 12 | -4 | 5 | 35 | 25 | 9 | 2 | 2 | 5 | 398 | 399 | 4 | 31 | 32 | 18 | -4 | -3 | 6 | 64 | 66 | 4 | -3 | 3 | 6 | 57 | 62 | 3 |
| 13 | -4 | 5 | 315 | 305 | 7 | 2 | 2 | 5 | 326 | 317 | 3 | 21 | 7 | 20 | -3 | -3 | 6 | 90 | 98 | 3 | -2 | 3 | 6 | 308 | 298 | 5 |
| 14 | -4 | 5 | 51 | 61 | 4 | 2 | 2 | 5 | 48 | 47 | 2 | 25 | 13 | 18 | -2 | -3 | 6 | 9 | 11 | 9 | -1 | 3 | 6 | 12 | 4 | 11 |
| 15 | -4 | 5 | 326 | 296 | 4 | 2 | 2 | 5 | 48 | 42 | 0 | 45 | 41 | 7 | -1 | -3 | 6 | 139 | 128 | 0 | 0 | 0 | 6 | 247 | 253 | 3 |
| 16 | -4 | 5 | 94 | 89 | 3 | 2 | 2 | 5 | 50 | 55 | 4 | 0 | 6 | 1 | 0 | -3 | 6 | 155 | 151 | 3 | 3 | 3 | 6 | 23 | 28 | 7 |
| 17 | -4 | 5 | 319 | 312 | 3 | 2 | 2 | 5 | 22 | 13 | 21 | 19 | 2 | 18 | 1 | -3 | 6 | 98 | 99 | 1 | 2 | 3 | 6 | 53 | 64 | 4 |
| 18 | -4 | 5 | 202 | 188 | 5 | 2 | 2 | 5 | 9 | 19 | 9 | 68 | 72 | 6 | 2 | -3 | 6 | 61 | 55 | 3 | 4 | 3 | 6 | 52 | 49 | 5 |
| 19 | -4 | 5 | 45 | 53 | 2 | 2 | 2 | 5 | 0 | 0 | 1 | 42 | 44 | 11 | 3 | -3 | 6 | 94 | 94 | 2 | 5 | 5 | 6 | 28 | 23 | 15 |
| 20 | -4 | 5 | 123 | 121 | 9 | 2 | 2 | 5 | 0 | 15 | 1 | 20 | 20 | 2 | 4 | -3 | 6 | 117 | 117 | 3 | 6 | 3 | 6 | 30 | 21 | 14 |
| 21 | -4 | 5 | 86 | 82 | 3 | 2 | 2 | 5 | 27 | 20 | 14 | 27 | 16 | 14 | 5 | -3 | 6 | 95 | 87 | 3 | -7 | 4 | 6 | 41 | 38 | 7 |
| 22 | -4 | 5 | 0 | 11 | 1 | 2 | 2 | 5 | 19 | 18 | 18 | 0 | -10 | 6 | 6 | 6 | 62 | 63 | 4 | -6 | 4 | 6 | 102 | 96 | 3 | |
| 23 | -4 | 5 | 24 | 26 | 23 | 2 | 2 | 5 | 42 | 42 | 6 | 98 | 96 | 3 | 7 | -3 | 6 | 17 | 11 | 16 | -5 | 4 | 6 | 72 | 75 | 3 |
| 24 | -4 | 5 | 39 | 37 | 8 | 2 | 2 | 5 | 105 | 105 | 2 | 12 | 16 | 12 | -7 | -2 | 6 | 32 | 18 | 6 | -4 | 4 | 6 | 64 | 63 | 4 |
| 25 | -4 | 5 | 17 | 26 | 17 | 2 | 2 | 5 | 221 | 218 | 5 | 27 | 39 | 26 | -6 | -2 | 6 | 12 | 3 | 11 | -3 | 4 | 6 | 24 | 17 | 12 |
| 26 | -4 | 5 | 35 | 47 | 8 | 2 | 2 | 5 | 341 | 347 | 5 | 0 | 6 | 6 | -5 | -2 | 6 | 38 | 35 | 7 | -1 | 4 | 6 | 84 | 81 | 1 |
| 27 | -4 | 5 | 119 | 117 | 2 | 2 | 2 | 5 | 186 | 187 | 2 | 33 | 21 | 17 | -4 | -2 | 6 | 196 | 227 | 7 | 0 | 4 | 6 | 407 | 402 | 4 |
| 28 | -4 | 5 | 141 | 164 | 6 | 2 | 2 | 5 | 99 | 96 | 1 | 52 | 55 | 8 | -3 | -2 | 6 | 34 | 24 | 6 | 1 | 4 | 6 | 101 | 108 | 6 |
| 29 | -4 | 5 | 552 | 545 | 1 | 2 | 2 | 5 | 199 | 214 | 4 | 105 | 101 | 3 | -2 | -2 | 6 | 494 | 467 | 6 | 2 | 4 | 6 | 42 | 40 | 6 |
| 30 | -4 | 5 | 195 | 212 | 3 | 2 | 2 | 5 | 50 | 50 | 5 | 19 | 14 | 18 | -1 | -2 | 6 | 154 | 165 | 2 | 3 | 4 | 6 | 89 | 103 | 3 |
| 31 | -4 | 5 | 175 | 159 | 6 | 2 | 2 | 5 | 136 | 150 | 5 | 17 | 25 | 17 | 0 | -2 | 6 | 187 | 185 | 3 | 4 | 4 | 6 | 2 | 21 | 2 |
| 32 | -4 | 5 | 555 | 563 | 4 | 2 | 2 | 5 | 24 | 23 | 20 | 46 | 41 | 8 | 1 | -2 | 6 | 129 | 133 | 2 | 5 | 4 | 6 | 19 | 1 | 19 |
| 33 | -4 | 5 | 0 | 1 | 1 | 2 | 2 | 5 | 41 | 38 | 9 | 72 | 76 | 5 | 2 | -2 | 6 | 57 | 34 | 3 | 6 | 4 | 6 | 0 | 1 | 1 |
| 34 | -4 | 5 | 31 | 29 | 8 | 2 | 2 | 5 | 16 | 1 | 16 | 0 | 4 | 1 | 3 | -2 | 6 | 112 | 109 | 3 | -7 | 5 | 6 | 48 | 40 | 7 |
| 35 | -4 | 5 | 95 | 82 | 3 | 2 | 2 | 5 | 34 | 20 | 10 | 82 | 83 | 5 | 4 | -2 | 6 | 169 | 166 | 4 | -6 | 5 | 6 | 24 | 25 | 18 |
| 36 | -4 | 5 | 34 | 32 | 8 | 2 | 2 | 5 | 4 | 6 | 3 | 46 | 42 | 10 | -4 | -8 | 6 | 58 | 54 | 10 | -5 | 5 | 6 | 125 | 120 | 3 |
| 37 | -4 | 5 | 48 | 31 | 7 | 2 | 2 | 5 | 52 | 53 | 5 | 58 | 52 | 7 | -3 | -8 | 6 | 42 | 40 | 7 | -4 | 5 | 6 | 154 | 156 | 4 |
| 38 | -4 | 5 | 31 | 20 | 13 | 2 | 2 | 5 | 80 | 72 | 3 | 23 | 13 | 22 | -2 | -8 | 6 | 23 | 13 | 22 | -3 | 5 | 6 | 135 | 142 | 3 |
| 39 | -4 | 5 | 21 | 14 | 20 | 2 | 2 | 5 | 134 | 133 | 3 | 22 | 5 | 21 | -7 | -1 | 6 | 9 | 17 | 8 | -2 | 5 | 6 | 15 | 14 | 14 |
| 40 | -4 | 5 | 115 | 129 | 5 | 2 | 2 | 5 | 146 | 152 | 3 | 119 | 115 | 2 | -6 | -1 | 6 | 58 | 62 | 5 | -1 | 5 | 6 | 15 | 22 | 15 |
| 41 | -4 | 5 | 111 | 109 | 2 | 2 | 2 | 5 | 431 | 429 | 4 | 171 | 163 | 7 | -4 | -1 | 6 | 35 | 38 | 7 | 0 | 6 | 6 | 0 | 0 | 1 |
| 42 | -4 | 5 | 182 | 183 | 4 | 2 | 2 | 5 | 65 | 65 | 2 | 90 | 100 | 4 | -4 | -1 | 6 | 195 | 187 | 4 | 1 | 1 | 6 | 0 | 12 | 1 |
| 43 | -4 | 5 | 41 | 48 | 4 | 2 | 2 | 5 | 178 | 182 | 6 | 52 | 54 | 7 | -3 | -1 | 6 | 122 | 141 | 4 | 2 | 2 | 6 | 66 | 72 | 4 |
| 44 | -4 | 5 | 58 | 61 | 2 | 2 | 2 | 5 | 20 | 20 | 20 | 12 | 22 | 11 | 1 | -1 | 6 | 52 | 56 | 3 | 3 | 3 | 6 | 0 | 5 | 1 |
| 45 | -4 | 5 | 269 | 273 | 2 | 2 | 2 | 5 | 19 | 25 | 18 | 47 | 68 | 8 | -2 | -1 | 6 | 488 | 492 | 3 | 4 | 4 | 6 | 34 | 36 | 11 |
| 46 | -4 | 5 | 58 | 62 | 1 | 2 | 2 | 5 | 45 | 45 | 6 | 31 | 26 | 16 | 0 | 0 | 6 | 349 | 350 | 3 | 5 | 5 | 6 | 32 | 15 | 13 |
| 47 | -4 | 5 | 75 | 75 | 2 | 2 | 2 | 5 | 59 | 52 | 8 | 9 | 9 | 9 | -1 | -1 | 6 | 303 | 318 | 5 | -7 | 6 | 6 | 21 | 28 | 20 |
| 48 | -4 | 5 | 233 | 219 | 5 | 2 | 2 | 5 | 16 | 14 | 15 | 26 | 19 | 25 | -4 | -7 | 6 | 255 | 265 | 5 | -5 | 6 | 6 | 0 | 3 | 1 |
| 49 | -4 | 5 | 253 | 254 | 6 | 2 | 2 | 5 | 62 | 61 | 5 | 36 | 37 | 11 | -3 | -7 | 6 | 73 | 66 | 6 | -4 | 6 | 6 | 49 | 46 | 6 |
| 50 | -4 | 5 | 97 | 94 | 2 | 2 | 2 | 5 | 26 | 27 | 15 | 45 | 44 | 8 | 4 | -1 | 6 | 94 | 91 | 2 | -4 | 6 | 6 | 120 | 125 | 5 |
| 51 | -4 | 5 | 15 | 7 | 14 | 2 | 2 | 5 | 89 | 90 | 3 | 25 | 29 | 24 | 5 | -1 | 6 | 40 | 43 | 6 | -3 | 6 | 6 | 45 | 53 | 4 |
| 52 | -4 | 5 | 26 | 19 | 15 | 2 | 2 | 5 | 179 | 183 | 4 | 72 | 65 | 3 | 6 | -1 | 6 | 25 | 19 | 20 | -1 | 6 | 6 | 232 | 237 | 4 |
| 53 | -4 | 5 | 12 | 8 | 11 | 2 | 2 | 5 | 42 | 34 | 7 | 186 | 183 | 4 | -7 | 0 | 6 | 5 | 27 | 4 | 0 | 6 | 6 | 45 | 47 | 5 |
| 54 | -4 | 5 | 56 | 42 | 4 | 2 | 2 | 5 | 68 | 67 | 3 | 38 | 27 | 9 | -6 | 0 | 6 | 32 | 32 | 9 | 1 | 6 | 6 | 89 | 94 | 4 |
| 55 | -4 | 5 | 110 | 115 | 4 | 2 | 2 | 5 | 53 | 58 | 4 | 30 | 37 | 14 | -5 | 0 | 6 | 60 | 57 | 4 | 3 | 6 | 6 | 63 | 64 | 6 |
| 56 | -4 | 5 | 100 | 99 | 2 | 2 | 2 | 5 | 40 | 37 | 9 | 64 | 75 | 5 | -4 | 0 | 6 | 68 | 71 | 3 | 4 | 6 | 6 | 57 | 51 | 7 |
| 57 | -4 | 5 | 66 | 63 | 2 | 2 | 2 | 5 | 78 | 92 | 5 | 42 | 36 | 10 | -3 | 0 | 6 | 147 | 155 | 4 | 4 | 6 | 6 | 0 | 10 | 1 |
| 58 | -4 | 5 | 311 | 325 | 2 | 2 | 2 | 5 | 39 | 21 | 10 | 44 | 40 | 6 | -2 | 0 | 6 | 54 | 56 | 3 | -7 | 7 | 6 | 0 | 2 | 1 |
| 59 | -4 | 5 | 203 | 197 | 9 | 2 | 2 | 5 | 34 | 28 | 14 | 64 | 61 | 9 | -1 | 0 | 6 | 96 | 81 | 4 | 6 | 6 | 6 | 38 | 35 | 4 |
| 60 | -4 | 5 | 496 | 526 | 3 | 2 | 2 | 5 | 0 | 0 | 1 | 0 | 6 | 1 | 0 | 0 | 6 | 245 | 254 | 3 | -5 | 7 | 6 | 72 | 62 | 10 |
| 61 | -4 | 5 | 21 | 20 | 9 | 2 | 2 | 5 | 13 | 17 | 13 | 99 | 104 | 3 | 2 | 0 | 6 | 491 | 491 | 4 | -4 | 7 | 6 | 26 | 22 | 16 |
| 62 | -4 | 5 | 86 | 92 | 2 | 2 | 2 | 5 | 21 | 15 | 20 | 195 | 179 | 4 | -1 | -6 | 6 | 520 | 532 | 4 | -3 | 7 | 6 | 27 | 19 | 15 |
| 63 | -4 | 5 | 154 | 160 | 4 | 2 | 2 | 5 | 0 | 2 | 1 | 132 | 131 | 2 | 3 | 0 | 6 | 201 | 213 | 6 | -3 | 7 | 6 | 27 | 19 | 15 |
| 64 | -4 | 5 | 80 | 81 | 3 | 2 | 2 | 5 | 37 | 43 | 9 | 115 | 120 | 2 | 4 | 0 | 6 | 208 | 202 | 4 | -1 | 7 | 6 | 136 | 150 | 4 |
| 65 | -4 | 5 | 4 | 11 | 3 | 2 | 2 | 5 | 30 | 4 | 13 | 119 | 108 | 3 | 5 | 0 | 6 | 31 | 25 | 9 | -1 | 7 | 6 | 113 | 112 | 2 |
| 66 | -4 | 5 | 46 | 34 | 8 | 2 | 2 | 5 | 28 | 20 | 15 | 70 | 66 | 4 | 6 | 0 | 6 | 34 | 24 | 9 | 0 | 7 | 6 | 148 | 139 | 2 |
| 67 | -4 | 5 | 21 | 23 | 10 | 2 | 2 | 5 | 107 | 98 | 2 | 130 | 131 | 3 | 7 | 0 | 6 | 21 | 17 | 21 | 1 | 7 | 6 | 145 | 145 | 5 |
| 68 | -4 | 5 | 25 | 10 | 13 | 2 | 2 | 5 | 171 | 166 | 12 | 32 | 27 | 12</ | | | | | | | | | | | | |

Table 1. Observed and calculated structure factors for 1

| h k l | | | 10Fo | | | 10Fc | | | 10s | | | h k l | | | 10Fo | | | 10Fc | | | 10s | | | h k l | | | 10Fo | | | 10Fc | | | 10s | | |
|-------|----|---|------|-----|----|------|----|---|-----|-----|----|-------|---|---|------|-----|----|------|----|---|-----|-----|----|-------|----|---|------|-----|----|------|--|--|-----|--|--|
| -4 | 10 | 6 | 74 | 80 | 5 | -3 | -3 | 7 | 68 | 76 | 4 | -1 | 3 | 7 | 269 | 285 | 3 | -1 | -9 | 8 | 9 | 13 | 8 | 3 | -2 | 8 | 188 | 184 | 4 | | | | | | |
| -3 | 10 | 6 | 57 | 56 | 7 | -2 | -3 | 7 | 48 | 46 | 5 | 0 | 3 | 7 | 18 | 15 | 10 | 0 | -9 | 8 | 23 | 25 | 18 | 4 | -2 | 8 | 60 | 50 | 4 | | | | | | |
| -2 | 10 | 6 | 33 | 6 | 14 | -1 | -3 | 7 | 116 | 112 | 1 | 1 | 1 | 7 | 0 | 13 | 1 | 1 | -9 | 8 | 0 | 11 | 1 | 5 | -2 | 8 | 0 | 18 | 1 | | | | | | |
| -1 | 10 | 6 | 79 | 80 | 10 | 0 | -3 | 7 | 79 | 75 | 2 | 2 | 2 | 7 | 97 | 100 | 3 | 2 | -9 | 8 | 19 | 33 | 18 | 6 | -2 | 8 | 54 | 47 | 5 | | | | | | |
| 0 | 10 | 6 | 10 | 10 | 13 | 0 | -3 | 7 | 239 | 243 | 3 | 3 | 3 | 7 | 87 | 87 | 3 | 3 | -9 | 8 | 78 | 77 | 5 | 7 | -2 | 8 | 0 | 1 | 1 | | | | | | |
| 1 | 10 | 6 | 18 | 22 | 12 | 2 | -3 | 7 | 143 | 148 | 3 | 4 | 4 | 7 | 44 | 37 | 7 | 4 | -9 | 8 | 47 | 41 | 8 | -1 | -2 | 8 | 0 | 11 | 1 | | | | | | |
| -3 | 11 | 6 | 39 | 45 | 12 | 5 | -3 | 7 | 20 | 12 | 20 | 5 | 5 | 7 | 57 | 48 | 6 | 5 | -9 | 8 | 46 | 47 | 9 | -6 | -1 | 8 | 25 | 18 | 18 | | | | | | |
| -2 | 11 | 6 | 21 | 0 | 20 | 4 | -3 | 7 | 96 | 97 | 3 | 6 | 6 | 7 | 22 | 10 | 22 | -4 | -8 | 8 | 11 | 22 | 10 | -5 | -1 | 8 | 60 | 58 | 4 | | | | | | |
| -1 | 11 | 6 | 32 | 16 | 15 | 5 | -3 | 7 | 39 | 34 | 7 | -7 | 4 | 7 | 45 | 42 | 7 | -3 | -8 | 8 | 16 | 6 | 16 | -4 | -1 | 8 | 195 | 212 | 5 | | | | | | |
| 1 | 11 | 6 | 0 | 10 | 1 | 6 | -3 | 7 | 21 | 19 | 20 | -6 | 4 | 7 | 82 | 76 | 3 | -2 | -8 | 8 | 24 | 26 | 23 | -3 | -1 | 8 | 112 | 116 | 3 | | | | | | |
| -2 | 11 | 7 | 25 | 19 | 25 | 7 | -3 | 7 | 58 | 41 | 10 | -5 | 4 | 7 | 50 | 45 | 5 | -1 | -8 | 8 | 16 | 25 | 15 | -2 | -1 | 8 | 55 | 60 | 3 | | | | | | |
| -1 | 11 | 7 | 0 | 10 | 1 | -7 | -2 | 7 | 37 | 28 | 10 | -4 | 4 | 7 | 110 | 114 | 2 | 0 | -8 | 8 | 78 | 80 | 4 | 0 | -1 | 8 | 388 | 413 | 3 | | | | | | |
| 0 | 11 | 7 | 21 | 8 | 29 | -6 | -2 | 7 | 30 | 28 | 12 | -3 | 4 | 7 | 49 | 48 | 4 | 1 | -8 | 8 | 66 | 53 | 5 | 1 | -1 | 8 | 154 | 142 | 3 | | | | | | |
| -1 | 10 | 7 | 21 | 11 | 21 | -5 | -2 | 7 | 56 | 58 | 5 | -2 | 4 | 7 | 129 | 119 | 3 | 2 | -8 | 8 | 48 | 53 | 5 | 2 | -1 | 8 | 75 | 78 | 2 | | | | | | |
| 1 | 10 | 7 | 28 | 23 | 13 | -4 | -2 | 7 | 62 | 67 | 4 | -1 | 4 | 7 | 107 | 118 | 2 | 3 | -8 | 8 | 66 | 59 | 5 | 1 | -1 | 8 | 29 | 29 | 9 | | | | | | |
| 2 | 10 | 7 | 33 | 10 | 14 | -3 | -2 | 7 | 87 | 93 | 4 | 0 | 4 | 7 | 200 | 206 | 4 | 4 | -8 | 8 | 32 | 29 | 13 | 3 | -1 | 8 | 90 | 79 | 3 | | | | | | |
| 3 | 10 | 7 | 0 | 6 | 1 | -2 | -2 | 7 | 129 | 136 | 4 | 1 | 4 | 7 | 79 | 88 | 2 | 5 | -8 | 8 | 72 | 79 | 14 | 5 | -1 | 8 | 75 | 67 | 3 | | | | | | |
| -4 | 10 | 7 | 77 | 88 | 6 | 0 | -2 | 7 | 290 | 280 | 3 | 2 | 4 | 7 | 34 | 41 | 9 | -4 | -7 | 8 | 34 | 36 | 14 | -7 | -1 | 8 | 18 | 6 | 17 | | | | | | |
| -3 | 9 | 7 | 0 | 5 | 1 | -1 | -2 | 7 | 199 | 183 | 8 | 3 | 4 | 7 | 0 | 13 | 1 | -3 | -7 | 8 | 25 | 25 | 25 | -1 | -1 | 8 | 7 | 2 | 6 | | | | | | |
| -2 | 9 | 7 | 27 | 45 | 27 | 0 | -2 | 7 | 37 | 33 | 3 | 4 | 4 | 7 | 3 | 13 | 2 | -2 | -7 | 8 | 100 | 98 | 4 | 7 | 0 | 8 | 31 | 22 | 10 | | | | | | |
| -1 | 9 | 7 | 52 | 47 | 5 | 1 | -2 | 7 | 54 | 53 | 3 | 5 | 4 | 7 | 11 | 17 | 11 | -1 | -7 | 8 | 103 | 103 | 2 | -6 | 0 | 8 | 28 | 20 | 10 | | | | | | |
| 0 | 9 | 7 | 72 | 72 | 4 | 4 | -2 | 7 | 63 | 60 | 3 | -7 | 5 | 7 | 39 | 27 | 8 | 0 | -7 | 8 | 29 | 30 | 2 | -5 | 0 | 8 | 333 | 315 | 6 | | | | | | |
| 1 | 9 | 7 | 0 | 1 | 1 | 3 | -2 | 7 | 43 | 41 | 6 | -6 | 5 | 7 | 42 | 42 | 7 | 1 | -7 | 8 | 22 | 16 | 16 | -4 | 0 | 8 | 75 | 79 | 3 | | | | | | |
| 2 | 9 | 7 | 8 | 29 | 8 | 5 | -2 | 7 | 35 | 22 | 8 | -5 | 5 | 7 | 69 | 67 | 4 | 2 | -7 | 8 | 6 | 6 | 5 | -3 | 0 | 8 | 211 | 214 | 5 | | | | | | |
| 3 | 9 | 7 | 48 | 52 | 8 | 6 | -2 | 7 | 24 | 18 | 15 | -4 | 5 | 7 | 0 | 0 | 1 | 3 | -7 | 8 | 74 | 79 | 4 | -1 | 0 | 8 | 72 | 62 | 2 | | | | | | |
| 4 | 9 | 7 | 52 | 60 | 7 | 7 | -2 | 7 | 0 | 2 | 1 | -3 | 5 | 7 | 0 | 3 | 1 | 4 | -7 | 8 | 71 | 74 | 5 | 0 | 0 | 8 | 74 | 63 | 1 | | | | | | |
| 5 | 9 | 7 | 14 | 22 | 14 | -7 | -1 | 7 | 0 | 7 | 1 | -2 | 5 | 7 | 20 | 17 | 19 | 5 | -7 | 8 | 63 | 56 | 6 | 0 | 0 | 8 | 236 | 251 | 3 | | | | | | |
| -4 | 8 | 7 | 22 | 22 | 22 | -6 | -1 | 7 | 46 | 43 | 6 | -1 | 5 | 7 | 110 | 109 | 1 | -5 | -6 | 8 | 17 | 9 | 16 | -5 | 0 | 8 | 140 | 146 | 3 | | | | | | |
| -3 | 8 | 7 | 82 | 87 | 5 | -5 | -1 | 7 | 39 | 51 | 7 | 0 | 0 | 7 | 134 | 131 | 2 | -4 | -6 | 8 | 25 | 17 | 25 | 3 | 0 | 8 | 129 | 137 | 4 | | | | | | |
| -2 | 8 | 7 | 20 | 30 | 19 | -4 | -1 | 7 | 177 | 162 | 4 | 1 | 1 | 7 | 145 | 144 | 3 | -3 | -6 | 8 | 60 | 56 | 6 | 4 | 0 | 8 | 28 | 30 | 11 | | | | | | |
| -1 | 8 | 7 | 12 | 3 | 12 | -3 | -1 | 7 | 241 | 239 | 5 | 2 | 2 | 7 | 50 | 42 | 6 | -2 | -6 | 8 | 38 | 42 | 10 | -5 | 0 | 8 | 133 | 127 | 4 | | | | | | |
| 0 | 8 | 7 | 125 | 122 | 2 | -2 | -1 | 7 | 309 | 327 | 5 | 3 | 3 | 7 | 28 | 26 | 16 | -2 | -6 | 8 | 104 | 103 | 3 | 5 | 0 | 8 | 0 | 12 | 1 | | | | | | |
| 1 | 8 | 7 | 98 | 104 | 3 | -1 | -1 | 7 | 118 | 107 | 2 | -7 | 6 | 7 | 31 | 12 | 13 | 1 | -6 | 8 | 319 | 317 | 5 | -7 | 1 | 8 | 68 | 68 | 4 | | | | | | |
| 2 | 8 | 7 | 14 | 14 | 13 | 0 | -1 | 7 | 182 | 179 | 3 | -6 | 6 | 7 | 48 | 45 | 6 | 2 | -6 | 8 | 18 | 14 | 18 | -6 | 1 | 8 | 123 | 126 | 2 | | | | | | |
| 3 | 8 | 7 | 100 | 101 | 4 | 1 | -1 | 7 | 185 | 180 | 3 | -7 | 6 | 7 | 31 | 12 | 13 | 1 | -6 | 8 | 231 | 238 | 5 | -6 | 1 | 8 | 59 | 50 | 4 | | | | | | |
| 4 | 8 | 7 | 93 | 90 | 4 | 2 | -1 | 7 | 144 | 140 | 3 | -6 | 6 | 7 | 48 | 45 | 6 | 3 | -6 | 8 | 18 | 14 | 18 | -4 | 1 | 8 | 105 | 97 | 2 | | | | | | |
| 5 | 8 | 7 | 13 | 4 | 13 | 3 | -1 | 7 | 287 | 294 | 6 | -5 | 6 | 7 | 0 | 8 | 1 | 4 | -6 | 8 | 69 | 73 | 4 | -4 | 1 | 8 | 11 | 11 | 10 | | | | | | |
| -5 | 7 | 7 | 55 | 53 | 9 | 4 | -1 | 7 | 33 | 31 | 8 | -4 | 6 | 7 | 22 | 4 | 22 | 3 | -6 | 8 | 43 | 42 | 8 | -2 | 1 | 8 | 152 | 155 | 2 | | | | | | |
| -4 | 7 | 7 | 46 | 40 | 9 | 5 | -1 | 7 | 45 | 41 | 5 | -3 | 6 | 7 | 286 | 284 | 6 | -3 | -6 | 8 | 38 | 30 | 10 | -1 | 1 | 8 | 259 | 273 | 3 | | | | | | |
| -3 | 7 | 7 | 39 | 40 | 10 | 6 | -1 | 7 | 32 | 27 | 10 | -2 | 6 | 7 | 166 | 172 | 3 | 6 | -6 | 8 | 68 | 59 | 5 | -1 | 1 | 8 | 472 | 500 | 3 | | | | | | |
| -2 | 7 | 7 | 0 | 4 | 1 | -1 | -1 | 7 | 23 | 16 | 22 | -1 | 6 | 7 | 196 | 208 | 3 | -6 | -6 | 8 | 12 | 8 | 11 | 0 | 1 | 8 | 101 | 102 | 2 | | | | | | |
| -1 | 7 | 7 | 138 | 139 | 2 | -7 | 0 | 7 | 30 | 22 | 12 | 0 | 6 | 7 | 217 | 206 | 3 | -5 | -5 | 8 | 83 | 90 | 4 | 1 | 1 | 8 | 29 | 32 | 10 | | | | | | |
| 0 | 7 | 7 | 35 | 34 | 11 | -6 | 0 | 7 | 42 | 41 | 6 | 1 | 6 | 7 | 76 | 77 | 3 | -4 | -5 | 8 | 0 | 8 | 1 | 3 | 1 | 8 | 13 | 16 | 13 | | | | | | |
| 1 | 7 | 7 | 136 | 132 | 2 | -5 | 0 | 7 | 170 | 153 | 4 | 2 | 6 | 7 | 100 | 97 | 3 | -3 | -5 | 8 | 121 | 132 | 3 | 4 | 4 | 8 | 40 | 36 | 7 | | | | | | |
| 2 | 7 | 7 | 236 | 231 | 5 | -4 | 0 | 7 | 90 | 98 | 3 | 3 | 6 | 7 | 61 | 56 | 6 | -2 | -5 | 8 | 31 | 28 | 7 | 5 | 5 | 8 | 45 | 38 | 7 | | | | | | |
| 3 | 7 | 7 | 8 | 8 | 3 | -3 | 0 | 7 | 152 | 148 | 5 | 4 | 6 | 7 | 0 | 3 | 11 | 1 | -5 | 8 | 12 | 9 | 11 | -6 | 6 | 8 | 26 | 5 | 14 | | | | | | |
| 4 | 7 | 7 | 81 | 84 | 4 | -2 | -1 | 7 | 308 | 317 | 5 | 5 | 6 | 7 | 40 | 19 | 3 | 0 | -5 | 8 | 70 | 69 | 4 | -7 | 1 | 8 | 50 | 46 | 5 | | | | | | |
| 5 | 7 | 7 | 33 | 24 | 12 | -1 | 0 | 7 | 400 | 425 | 3 | -6 | 7 | 7 | 48 | 38 | 7 | 1 | -5 | 8 | 181 | 182 | 3 | -6 | 2 | 8 | 98 | 89 | 3 | | | | | | |
| -5 | 6 | 7 | 19 | 5 | 18 | 0 | 0 | 7 | 217 | 235 | 3 | -5 | 7 | 7 | 39 | 35 | 9 | 3 | -5 | 8 | 95 | 95 | 3 | -5 | 2 | 8 | 82 | 77 | 3 | | | | | | |
| -4 | 6 | 7 | 3 | 3 | 3 | 1 | 1 | 7 | 615 | 638 | 7 | -4 | 7 | 7 | 77 | 73 | 4 | 4 | -5 | 8 | 112 | 112 | 3 | -4 | 2 | 8 | 34 | 27 | 6 | | | | | | |
| -3 | 6 | 7 | 22 | 15 | 21 | 2 | 0 | 7 | 175 | 170 | 4 | -3 | 7 | 7 | 25 | 24 | 18 | 5 | -5 | 8 | 86 | 85 | 4 | -3 | 2 | 8 | 91 | 103 | 2 | | | | | | |
| -2 | 6 | 7 | 46 | 46 | 7 | 3 | 0 | 7 | 83 | 76 | 4 | -2 | 7 | 7 | 103 | 105 | 3 | -6 | -5 | 8 | 0 | 9 | 1 | -2 | 2 | 8 | 49 | 41 | 2 | | | | | | |
| -1 | 6 | 7 | 143 | 154 | 4 | 4 | 0 | 7 | 97 | 99 | 3 | -1 | 7 | 7 | 84 | 85 | 2 | -6 | -4 | 8 | 9 | 9 | 8 | -1 | 2 | 8 | 300 | 314 | 4 | | | | | | |
| 0 | 6 | 7 | 327 | 323 | 5 | 5 | 0 | 7 | 57 | 49 | 4 | 0 | 7 | 7 | 150 | 153 | 2 | -5 | -4 | 8 | 0 | 5 | 1 | 0 | 1 | 8 | 0 | 18 | 1 | | | | | | |
| 1 | 6 | 7 | 158 | 151 | 2 | 6 | 0 | 7 | 11 | 5 | 10 | 0 | 7 | 7 | 20 | 5 | 20 | 0 | -4 | 8 | 123 | 122 | 4 | 1 | 1 | 8 | 145 | 155 | 4 | | | | | | |
| 2 | 6 | 7 | 212 | 202 | 11 | 7 | 0 | 7 | 21 | 14 | 20 | 2 | 7 | 7 | 42 | 45 | 19 | -3 | -4 | 8 | 134 | 142 | 4 | 2 | 2 | 8 | 21 | 35 | 21 | | | | | | |
| 3 | 6 | 7 | 95 | 97 | 3 | -7 | 1 | 7 | 53 | 33 | 5 | -6 | 8 | 7 | 19 | 21 | 19 | -2 | -4 | 8 | 23 | 26 | 21 | 3 | 4 | 8 | 157 | 135 | 3 | | | | | | |
| 4 | 6 | 7 | 110 | 117 | 3 | -6 | 1 | 7 | 39 | 35 | 7 | -4 | 8 | 7 | 12 | 22 | 12 | 1 | -4 | 8 | 115 | 114 | 1 | 5 | 2 | 8 | 28 | 11 | 13 | | | | | | |
| 5 | 6 | 7 | 130 | 141 | 3 | -5 | 1 | 7 | 107 | 108 | 2 | -5 | 8 | 7 | 37 | 41 | 10 | 0 | -4 | 8 | 33 | 32 | 5 | 6 | 2 | 8 | 31 | 24 | 10 | | | | | | |
| -6 | 6 | 7 | 6 | 25 | 5 | -3 | 1 | 7 | 167 | 169 | 4 | -4 | 8 | 7 | 76 | 74 | 4 | 2 | -4 | 8 | 194 | 191 | 4 | -7 | 3 | 8 | 68 | 59 | 4 | | | | | | |
| -5 | 6 | 7 | 46 | 35 | 10 | -2 | 1 | 7 | 240 | 236 | 5 | -3 | 8 | 7 | 108 | 104 | 3 | 3 | -4 | 8 | 112 | 108 | 2 | -6 | 3 | 8 | 140 | 141 | 3 | | | | | | |
| -4 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

| Table 1. | | Observed and calculated structure factors for 1 | | | | | | | | | | | | | | | Page 6 | | | | | | |
|----------|----|---|------|------|-----|----|----|---|------|------|-----|----|---|---|------|------|--------|----|-----|----|------|------|-----|
| h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s | h | k | l | 10Fo | 10Fc | 10s |
| -5 | 5 | 5 | 34 | 33 | 8 | -3 | -6 | 9 | 104 | 101 | 3 | -6 | 1 | 9 | 25 | 25 | 14 | -4 | 8 | 9 | 83 | 97 | 4 |
| -4 | 5 | 8 | 92 | 97 | 3 | -2 | -6 | 9 | 17 | 20 | 16 | -5 | 1 | 9 | 0 | 3 | 1 | -3 | 8 | 9 | 62 | 58 | 5 |
| -3 | 5 | 8 | 17 | 21 | 16 | -1 | -6 | 9 | 63 | 61 | 3 | -4 | 1 | 9 | 75 | 80 | 3 | -1 | 8 | 9 | 21 | 21 | 21 |
| -2 | 5 | 8 | 85 | 89 | 3 | 0 | -6 | 9 | 180 | 179 | 3 | -3 | 1 | 9 | 174 | 177 | 4 | 0 | 8 | 9 | 33 | 19 | 8 |
| -1 | 5 | 8 | 43 | 51 | 4 | 1 | -6 | 9 | 146 | 153 | 2 | -2 | 1 | 9 | 293 | 302 | 5 | 1 | 8 | 8 | 29 | 35 | 10 |
| 0 | 5 | 8 | 290 | 279 | 4 | 2 | -6 | 9 | 82 | 80 | 4 | -1 | 1 | 9 | 251 | 264 | 7 | 2 | 8 | 8 | 0 | 11 | 1 |
| 1 | 5 | 8 | 31 | 36 | 7 | 3 | -6 | 9 | 97 | 99 | 3 | 0 | 1 | 9 | 57 | 56 | 2 | 3 | 8 | 8 | 15 | 5 | 14 |
| 2 | 5 | 8 | 94 | 94 | 3 | 4 | -6 | 9 | 90 | 87 | 4 | 1 | 1 | 9 | 118 | 111 | 2 | -5 | 9 | 9 | 0 | 3 | 1 |
| 3 | 5 | 8 | 75 | 68 | 4 | 5 | -6 | 9 | 57 | 57 | 6 | 2 | 1 | 9 | 22 | 28 | 15 | -4 | 9 | 9 | 44 | 45 | 9 |
| 4 | 5 | 8 | 12 | 3 | 11 | 6 | -6 | 9 | 12 | 22 | 12 | 3 | 1 | 9 | 108 | 97 | 2 | -3 | 9 | 9 | 18 | 8 | 17 |
| 5 | 5 | 8 | 31 | 16 | 16 | -5 | -5 | 9 | 56 | 62 | 7 | 4 | 1 | 9 | 79 | 78 | 3 | -2 | 9 | 9 | 36 | 30 | 11 |
| -7 | 6 | 6 | 19 | 28 | 19 | -4 | -5 | 9 | 57 | 54 | 6 | 5 | 1 | 9 | 52 | 50 | 5 | -1 | 9 | 9 | 15 | 4 | 15 |
| -6 | 6 | 6 | 41 | 31 | 8 | -3 | -5 | 9 | 37 | 44 | 9 | 6 | 1 | 9 | 26 | 26 | 19 | 0 | 9 | 9 | 0 | 0 | 1 |
| -5 | 6 | 6 | 65 | 64 | 4 | -2 | -5 | 9 | 78 | 75 | 4 | -7 | 2 | 9 | 40 | 28 | 7 | 1 | 9 | 9 | 31 | 28 | 10 |
| -4 | 6 | 6 | 52 | 56 | 5 | -1 | -5 | 9 | 131 | 129 | 3 | -6 | 2 | 9 | 41 | 47 | 7 | 2 | 9 | 9 | 0 | 1 | 1 |
| -3 | 6 | 6 | 49 | 48 | 6 | 0 | -5 | 9 | 137 | 143 | 2 | -5 | 2 | 9 | 82 | 82 | 3 | -4 | 10 | 9 | 53 | 43 | 8 |
| -2 | 6 | 6 | 98 | 84 | 3 | 1 | -5 | 9 | 124 | 128 | 2 | -4 | 2 | 9 | 108 | 108 | 2 | -3 | 10 | 9 | 84 | 88 | 5 |
| -1 | 6 | 6 | 134 | 128 | 2 | 2 | -5 | 9 | 169 | 176 | 4 | -3 | 2 | 9 | 67 | 69 | 3 | -2 | 10 | 9 | 35 | 46 | 14 |
| 0 | 6 | 6 | 21 | 13 | 18 | 3 | -5 | 9 | 0 | 8 | 1 | -2 | 2 | 9 | 182 | 198 | 4 | -1 | 10 | 9 | 40 | 38 | 8 |
| 1 | 6 | 6 | 17 | 8 | 16 | 4 | -5 | 9 | 38 | 42 | 9 | -1 | 2 | 9 | 148 | 143 | 3 | 0 | 10 | 9 | 59 | 54 | 5 |
| 2 | 6 | 6 | 30 | 18 | 13 | 5 | -5 | 9 | 58 | 56 | 6 | 0 | 2 | 9 | 36 | 40 | 4 | 0 | 10 | 10 | 0 | 11 | 1 |
| 3 | 6 | 6 | 0 | 15 | 1 | 6 | -5 | 9 | 20 | 33 | 19 | 1 | 2 | 9 | 36 | 31 | 4 | -1 | 10 | 10 | 50 | 53 | 6 |
| 4 | 6 | 6 | 40 | 44 | 10 | -6 | -4 | 9 | 0 | 13 | 1 | 2 | 2 | 9 | 22 | 18 | 16 | -2 | -10 | 10 | 20 | 12 | 20 |
| -6 | 7 | 7 | 21 | 22 | 21 | -5 | -4 | 9 | 37 | 36 | 9 | 3 | 2 | 9 | 58 | 55 | 4 | -2 | -9 | 10 | 0 | 13 | 1 |
| -4 | 7 | 7 | 45 | 39 | 7 | -4 | -4 | 9 | 0 | 9 | 1 | 4 | 2 | 9 | 25 | 36 | 15 | -1 | -9 | 10 | 31 | 23 | 11 |
| -3 | 7 | 7 | 33 | 32 | 11 | -3 | -4 | 9 | 62 | 64 | 5 | 5 | 2 | 9 | 58 | 59 | 10 | 0 | -9 | 10 | 41 | 40 | 7 |
| -2 | 7 | 7 | 27 | 24 | 15 | -2 | -4 | 9 | 33 | 24 | 9 | 6 | 3 | 9 | 37 | 31 | 10 | 1 | -9 | 10 | 0 | 8 | 1 |
| -1 | 7 | 7 | 32 | 26 | 11 | -1 | -4 | 9 | 132 | 133 | 2 | -7 | 3 | 9 | 23 | 17 | 22 | 2 | -9 | 10 | 39 | 32 | 11 |
| 0 | 7 | 7 | 28 | 22 | 9 | 0 | -4 | 9 | 14 | 27 | 14 | -6 | 3 | 9 | 64 | 63 | 4 | 3 | -9 | 10 | 67 | 66 | 6 |
| 1 | 7 | 7 | 27 | 34 | 10 | 1 | -4 | 9 | 214 | 220 | 12 | -5 | 3 | 9 | 32 | 24 | 9 | 4 | -9 | 10 | 22 | 18 | 22 |
| 2 | 7 | 7 | 22 | 29 | 17 | 2 | -4 | 9 | 43 | 36 | 6 | -4 | 3 | 9 | 125 | 130 | 2 | -3 | -8 | 10 | 34 | 41 | 14 |
| 3 | 7 | 7 | 61 | 66 | 6 | 3 | -4 | 9 | 142 | 152 | 3 | -3 | 3 | 9 | 18 | 1 | 17 | -2 | -8 | 10 | 140 | 143 | 3 |
| 4 | 7 | 7 | 59 | 60 | 7 | 4 | -4 | 9 | 108 | 103 | 3 | -2 | 3 | 9 | 88 | 89 | 2 | -1 | -8 | 10 | 13 | 7 | 12 |
| -6 | 8 | 8 | 29 | 33 | 23 | 5 | -4 | 9 | 25 | 30 | 17 | -1 | 3 | 9 | 82 | 72 | 2 | 0 | -8 | 10 | 59 | 57 | 4 |
| -5 | 8 | 8 | 28 | 18 | 18 | 6 | -4 | 9 | 4 | 2 | 4 | 0 | 3 | 9 | 93 | 89 | 2 | 1 | -8 | 10 | 74 | 73 | 3 |
| -4 | 8 | 8 | 18 | 18 | 17 | -6 | -3 | 9 | 67 | 51 | 5 | 1 | 3 | 9 | 107 | 110 | 1 | 2 | -8 | 10 | 57 | 53 | 6 |
| -3 | 8 | 8 | 68 | 73 | 5 | -5 | -3 | 9 | 82 | 77 | 4 | 2 | 3 | 9 | 73 | 75 | 4 | 3 | -8 | 10 | 0 | 13 | 1 |
| -2 | 8 | 8 | 80 | 72 | 4 | -4 | -3 | 9 | 61 | 63 | 4 | 3 | 3 | 9 | 49 | 56 | 5 | 4 | -8 | 10 | 72 | 78 | 5 |
| -1 | 8 | 8 | 111 | 105 | 3 | -3 | -3 | 9 | 39 | 43 | 7 | 4 | 3 | 9 | 46 | 48 | 7 | 5 | -8 | 10 | 24 | 24 | 24 |
| 0 | 8 | 8 | 99 | 106 | 2 | -1 | -3 | 9 | 185 | 186 | 3 | 5 | 3 | 9 | 30 | 28 | 14 | -4 | -7 | 10 | 57 | 53 | 7 |
| 1 | 8 | 8 | 86 | 87 | 3 | 0 | -3 | 9 | 18 | 27 | 14 | -7 | 4 | 9 | 0 | 11 | 1 | -3 | -7 | 10 | 61 | 72 | 7 |
| 2 | 8 | 8 | 14 | 4 | 13 | 1 | -3 | 9 | 86 | 89 | 2 | -6 | 4 | 9 | 22 | 21 | 22 | -2 | -7 | 10 | 66 | 67 | 5 |
| 3 | 8 | 8 | 19 | 2 | 18 | 2 | -3 | 9 | 36 | 36 | 7 | -5 | 4 | 9 | 94 | 84 | 3 | -1 | -7 | 10 | 82 | 83 | 3 |
| 4 | 8 | 8 | 40 | 27 | 11 | 3 | -3 | 9 | 232 | 223 | 5 | -4 | 4 | 9 | 27 | 31 | 12 | 0 | -7 | 10 | 70 | 71 | 3 |
| -5 | 9 | 9 | 71 | 71 | 5 | 4 | -3 | 9 | 52 | 46 | 5 | -3 | 4 | 9 | 121 | 126 | 2 | 1 | -7 | 10 | 99 | 102 | 2 |
| -4 | 9 | 9 | 17 | 28 | 17 | 5 | -3 | 9 | 24 | 14 | 17 | -2 | 4 | 9 | 69 | 77 | 3 | 2 | -7 | 10 | 23 | 11 | 22 |
| -3 | 9 | 9 | 89 | 95 | 4 | 6 | -3 | 9 | 43 | 33 | 7 | -1 | 4 | 9 | 206 | 211 | 3 | 3 | -7 | 10 | 142 | 144 | 3 |
| -2 | 9 | 9 | 5 | 13 | 4 | -7 | -2 | 9 | 12 | 2 | 12 | 0 | 4 | 9 | 216 | 212 | 3 | 4 | -7 | 10 | 22 | 4 | 21 |
| -1 | 9 | 9 | 50 | 51 | 5 | -6 | -2 | 9 | 59 | 52 | 5 | 1 | 4 | 9 | 294 | 283 | 5 | 5 | -7 | 10 | 8 | 15 | 8 |
| 0 | 9 | 9 | 29 | 29 | 11 | -5 | -2 | 9 | 21 | 9 | 21 | 5 | 4 | 9 | 37 | 51 | 9 | -5 | -6 | 10 | 46 | 39 | 9 |
| 1 | 9 | 9 | 40 | 42 | 8 | -4 | -2 | 9 | 13 | 18 | 13 | 4 | 4 | 9 | 84 | 87 | 4 | -4 | -6 | 10 | 46 | 46 | 8 |
| 2 | 9 | 9 | 21 | 10 | 21 | -3 | -2 | 9 | 95 | 96 | 3 | 4 | 4 | 9 | 34 | 32 | 10 | -3 | -6 | 10 | 20 | 22 | 20 |
| 3 | 9 | 9 | 14 | 32 | 14 | -2 | -2 | 9 | 86 | 82 | 2 | 5 | 4 | 9 | 27 | 30 | 19 | -2 | -6 | 10 | 28 | 16 | 16 |
| 4 | 9 | 9 | 25 | 30 | 25 | -1 | -2 | 9 | 340 | 348 | 4 | -7 | 5 | 9 | 82 | 66 | 4 | -1 | -6 | 10 | 48 | 52 | 4 |
| -10 | 10 | 10 | 0 | 4 | 1 | 0 | -2 | 9 | 374 | 392 | 3 | -6 | 5 | 9 | 37 | 34 | 8 | 0 | -6 | 10 | 170 | 167 | 2 |
| -9 | 10 | 10 | 47 | 46 | 8 | 1 | -2 | 9 | 17 | 12 | 13 | -5 | 5 | 9 | 32 | 3 | 3 | -1 | -6 | 10 | 74 | 77 | 5 |
| -8 | 10 | 10 | 51 | 44 | 6 | 2 | -2 | 9 | 0 | 11 | 1 | -4 | 5 | 9 | 118 | 113 | 2 | 2 | -6 | 10 | 20 | 3 | 20 |
| -7 | 10 | 10 | 7 | 2 | 6 | 3 | -2 | 9 | 197 | 195 | 4 | -3 | 5 | 9 | 170 | 168 | 3 | 3 | -6 | 10 | 92 | 94 | 3 |
| -6 | 10 | 10 | 17 | 24 | 16 | 4 | -2 | 9 | 124 | 124 | 3 | -2 | 5 | 9 | 180 | 198 | 4 | 4 | -6 | 10 | 28 | 30 | 16 |
| -5 | 10 | 10 | 45 | 43 | 7 | 5 | -2 | 9 | 82 | 69 | 3 | -1 | 5 | 9 | 143 | 147 | 2 | 5 | -6 | 10 | 53 | 68 | 7 |
| -4 | 10 | 10 | 40 | 41 | 11 | 6 | -2 | 9 | 42 | 31 | 8 | 0 | 5 | 9 | 143 | 141 | 2 | -5 | -6 | 10 | 15 | 21 | 15 |
| -3 | 10 | 10 | 0 | 18 | 1 | -7 | -1 | 9 | 11 | 11 | 10 | 1 | 5 | 9 | 22 | 28 | 13 | -4 | -5 | 10 | 76 | 80 | 5 |
| -2 | 10 | 10 | 0 | 9 | 1 | -6 | -1 | 9 | 30 | 28 | 12 | 2 | 5 | 9 | 70 | 65 | 4 | -3 | -5 | 10 | 13 | 4 | 12 |
| -1 | 10 | 10 | 111 | 107 | 2 | -5 | -1 | 9 | 106 | 106 | 4 | 3 | 5 | 9 | 14 | 11 | 14 | -2 | -5 | 10 | 121 | 110 | 3 |
| 0 | 10 | 10 | 103 | 102 | 4 | -4 | -1 | 9 | 31 | 32 | 10 | 4 | 5 | 9 | 18 | 17 | 17 | -1 | -5 | 10 | 180 | 181 | 3 |
| 1 | 10 | 10 | 11 | 7 | 10 | -3 | -1 | 9 | 272 | 270 | 6 | 5 | 5 | 9 | 34 | 29 | 13 | 0 | -5 | 10 | 136 | 132 | 2 |
| 2 | 10 | 10 | 12 | 9 | 11 | -2 | -1 | 9 | 133 | 143 | 3 | -7 | 6 | 9 | 17 | 27 | 17 | 1 | -5 | 10 | 120 | 119 | 2 |
| 3 | 10 | 10 | 44 | 50 | 10 | -1 | -1 | 9 | 84 | 90 | 1 | -6 | 6 | 9 | 86 | 79 | 4 | 2 | -5 | 10 | 56 | 57 | 5 |
| 4 | 10 | 10 | 52 | 54 | 8 | 0 | 0 | 9 | 63 | 66 | 2 | -5 | 6 | 9 | 36 | 39 | 8 | 3 | -5 | 10 | 20 | 8 | 19 |
| -8 | 8 | 9 | 37 | 27 | 12 | 1 | -1 | 9 | 232 | 240 | 4 | -4 | 6 | 9 | 22 | 26 | 22 | 4 | -5 | 10 | 112 | 118 | 3 |
| -7 | 8 | 9 | 106 | 105 | 4 | 2 | -1 | 9 | 35 | 33 | 6 | -3 | 6 | 9 | 53 | 56 | 5 | 5 | -5 | 10 | 136 | 130 | 3 |
| -6 | 8 | 9 | 13 | 14 | 13 | 3 | -1 | 9 | 0 | 2 | 1 | -2 | 6 | 9 | 76 | 75 | 4 | 6 | -5 | 10 | 29 | 18 | 16 |
| -5 | 8 | 9 | 48 | 41 | 5 | 4 | -1 | 9 | 0 | 1 | 1 | -1 | 6 | 9 | 0 | 2 | 1 | -6 | -4 | 10 | 24 | 23 | 23 |
| -4 | 8 | 9 | 86 | 82 | 3 | 5 | -1 | 9 | 39 | 31 | 7 | 0 | 6 | 9 | 17 | 30 | 16 | -5 | -4 | 10 | 13 | 20 | 12 |
| -3 | 8 | 9 | 15 | 18 | 14 | 6 | -1 | 9 | 21 | 3 | 21 | 1 | 6 | 9 | 32 | 40 | 7 | -4 | -4 | 10 | 0 | 10 | 1 |
| -2 | 8 | 9 | 23 | 30 | 22 | -7 | 0 | 9 | 26 | 28 | 1 | | | | | | | | | | | | |

| Table 1. | | Observed and calculated structure factors for 1 | | | | | | | | | | | | | | | Page 8 | | | | | | | | | | | | |
|----------|----|---|------|------|-----|----|----|----|------|------|-----|----|----|----|------|------|--------|----|----|----|------|------|-----|----|----|----|------|------|-----|
| 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 |
| -2 | -1 | 12 | 48 | 51 | 8 | 5 | -1 | 13 | 80 | 68 | 4 | 0 | 8 | 13 | 17 | 22 | 16 | -3 | 1 | 14 | 54 | 58 | 5 | -4 | -4 | 15 | 33 | 24 | 13 |
| -1 | 0 | 12 | 68 | 71 | 6 | -6 | 0 | 13 | 14 | 15 | 14 | 1 | 8 | 13 | 27 | 23 | 13 | -2 | 1 | 14 | 119 | 123 | 3 | -3 | -4 | 15 | 21 | 33 | 21 |
| 0 | 0 | 12 | 38 | 35 | 7 | -5 | 0 | 13 | 0 | 11 | 1 | -2 | 9 | 13 | 0 | 16 | 1 | -1 | 1 | 14 | 135 | 145 | 2 | -2 | -4 | 15 | 84 | 84 | 4 |
| 1 | 0 | 12 | 43 | 34 | 7 | -4 | 0 | 13 | 34 | 45 | 8 | -1 | -8 | 14 | 59 | 57 | 5 | 0 | 1 | 14 | 151 | 159 | 2 | -1 | -4 | 15 | 16 | 14 | 16 |
| 2 | 0 | 12 | 42 | 40 | 10 | -3 | 0 | 13 | 39 | 30 | 7 | 0 | -8 | 14 | 37 | 37 | 8 | 1 | 1 | 14 | 18 | 14 | 17 | 0 | -4 | 15 | 28 | 17 | 9 |
| 3 | 0 | 12 | 34 | 38 | 14 | -2 | 0 | 13 | 86 | 83 | 3 | 2 | -8 | 14 | 34 | 39 | 9 | 2 | 1 | 14 | 26 | 30 | 15 | 2 | -4 | 15 | 107 | 105 | 2 |
| 4 | 0 | 12 | 0 | 13 | 1 | -1 | 0 | 13 | 167 | 175 | 2 | 2 | -8 | 14 | 17 | 17 | 17 | 3 | 1 | 14 | 40 | 51 | 8 | 2 | -4 | 15 | 12 | 17 | 12 |
| 5 | 0 | 12 | 18 | 6 | 17 | 0 | 0 | 13 | 51 | 52 | 5 | -3 | -7 | 14 | 8 | 22 | 8 | 4 | 1 | 14 | 24 | 15 | 24 | 3 | -4 | 15 | 114 | 116 | 3 |
| 6 | 0 | 13 | 47 | 52 | 8 | 2 | 1 | 13 | 217 | 220 | 4 | -2 | -7 | 14 | 0 | 7 | 1 | -6 | 2 | 14 | 11 | 13 | 10 | 4 | -4 | 15 | 102 | 102 | 4 |
| 7 | 0 | 13 | 20 | 29 | 19 | 1 | 0 | 13 | 81 | 81 | 3 | -1 | -7 | 14 | 22 | 20 | 21 | -5 | 2 | 14 | 44 | 46 | 7 | -5 | -3 | 15 | 28 | 22 | 17 |
| 8 | 0 | 13 | 3 | 3 | 2 | 0 | 0 | 13 | 119 | 121 | 2 | 0 | 0 | 14 | 118 | 111 | 2 | -4 | 2 | 14 | 37 | 35 | 8 | -4 | -3 | 15 | 12 | 7 | 12 |
| 9 | 0 | 13 | 0 | 5 | 1 | 4 | 0 | 13 | 30 | 21 | 12 | 1 | -7 | 14 | 60 | 60 | 4 | -3 | 2 | 14 | 36 | 37 | 8 | -3 | -3 | 15 | 86 | 85 | 4 |
| 10 | 0 | 13 | 54 | 57 | 5 | 5 | 0 | 13 | 19 | 18 | 19 | 2 | -7 | 14 | 34 | 30 | 13 | -2 | 2 | 14 | 39 | 33 | 7 | -2 | -3 | 15 | 45 | 50 | 7 |
| 11 | 0 | 13 | 61 | 59 | 4 | -6 | 1 | 13 | 15 | 12 | 15 | 3 | -7 | 14 | 10 | 3 | 10 | -1 | 0 | 14 | 77 | 72 | 2 | 0 | -3 | 15 | 55 | 52 | 4 |
| 12 | 0 | 13 | 18 | 19 | 18 | -5 | 1 | 13 | 58 | 44 | 5 | -3 | -6 | 14 | 30 | 5 | 16 | 0 | 2 | 14 | 77 | 72 | 2 | 0 | -3 | 15 | 55 | 52 | 4 |
| 13 | 0 | 13 | 62 | 65 | 6 | -4 | 1 | 13 | 26 | 28 | 14 | -2 | -6 | 14 | 18 | 19 | 18 | 1 | 1 | 14 | 32 | 25 | 6 | 1 | -3 | 15 | 61 | 58 | 3 |
| 14 | 0 | 13 | 0 | 16 | 1 | -1 | 1 | 13 | 70 | 79 | 4 | -1 | -6 | 14 | 51 | 52 | 5 | 2 | 2 | 14 | 89 | 80 | 3 | 2 | -3 | 15 | 36 | 41 | 9 |
| 15 | 0 | 13 | 9 | 16 | 9 | -2 | 1 | 13 | 52 | 57 | 5 | 0 | -6 | 14 | 146 | 151 | 2 | 3 | 3 | 14 | 0 | 3 | 1 | 3 | -3 | 15 | 53 | 61 | 6 |
| 16 | 0 | 13 | 0 | 7 | 1 | -1 | 1 | 13 | 205 | 208 | 3 | 1 | -6 | 14 | 119 | 121 | 2 | -6 | 4 | 14 | 32 | 27 | 12 | -4 | -3 | 15 | 37 | 29 | 10 |
| 17 | 0 | 13 | 53 | 54 | 5 | 0 | 1 | 13 | 185 | 191 | 3 | 2 | -6 | 14 | 120 | 128 | 3 | -6 | 3 | 14 | 15 | 3 | 15 | -5 | -2 | 15 | 40 | 24 | 9 |
| 18 | 0 | 13 | 0 | 0 | 1 | 1 | 1 | 13 | 155 | 151 | 2 | 3 | -6 | 14 | 63 | 56 | 6 | -5 | 3 | 14 | 28 | 19 | 14 | -4 | -2 | 15 | 0 | 13 | 1 |
| 19 | 0 | 13 | 48 | 46 | 5 | 1 | 1 | 13 | 20 | 16 | 20 | 4 | -6 | 14 | 0 | 10 | 1 | -4 | 4 | 14 | 71 | 73 | 4 | -3 | -2 | 15 | 10 | 7 | 9 |
| 20 | 0 | 13 | 55 | 54 | 7 | 3 | 2 | 13 | 42 | 38 | 7 | -4 | -5 | 14 | 76 | 72 | 5 | -3 | 3 | 14 | 46 | 41 | 6 | -2 | -2 | 15 | 20 | 3 | 19 |
| 21 | 0 | 13 | 48 | 53 | 8 | 1 | 1 | 13 | 31 | 28 | 12 | -3 | -5 | 14 | 57 | 50 | 6 | -2 | 3 | 14 | 74 | 71 | 4 | -1 | -1 | 15 | 112 | 114 | 2 |
| 22 | 0 | 13 | 92 | 94 | 4 | 4 | 5 | 13 | 0 | 2 | 1 | -2 | -5 | 14 | 26 | 35 | 20 | -1 | 0 | 14 | 13 | 18 | 13 | 0 | -2 | 15 | 2 | 10 | 1 |
| 23 | 0 | 13 | 45 | 38 | 9 | -6 | 2 | 13 | 37 | 38 | 9 | -1 | -5 | 14 | 19 | 21 | 18 | 0 | 1 | 14 | 82 | 87 | 2 | 1 | -2 | 15 | 57 | 51 | 3 |
| 24 | 0 | 13 | 41 | 41 | 10 | -4 | 2 | 13 | 28 | 23 | 12 | 0 | -5 | 14 | 0 | 11 | 1 | 2 | 3 | 14 | 50 | 39 | 6 | 6 | -2 | 15 | 63 | 63 | 5 |
| 25 | 0 | 13 | 56 | 49 | 6 | -4 | 2 | 13 | 84 | 75 | 3 | 1 | -5 | 14 | 0 | 2 | 1 | 3 | 14 | 52 | 46 | 6 | 3 | -2 | 15 | 0 | 12 | 1 | 1 |
| 26 | 0 | 13 | 10 | 2 | 10 | -3 | 2 | 13 | 73 | 65 | 3 | 2 | -5 | 14 | 112 | 117 | 3 | 4 | 3 | 14 | 48 | 43 | 7 | 4 | -2 | 15 | 23 | 2 | 23 |
| 27 | 0 | 13 | 60 | 66 | 4 | -1 | 2 | 13 | 56 | 64 | 5 | -5 | -4 | 14 | 57 | 58 | 6 | -6 | 4 | 14 | 25 | 25 | 24 | -5 | -1 | 15 | 40 | 38 | 9 |
| 28 | 0 | 13 | 109 | 105 | 2 | 2 | 2 | 13 | 0 | 4 | 1 | -5 | -4 | 14 | 0 | 0 | 1 | -5 | 4 | 14 | 8 | 5 | 7 | -4 | -1 | 15 | 33 | 29 | 11 |
| 29 | 0 | 13 | 60 | 61 | 6 | 0 | 1 | 13 | 37 | 38 | 5 | -4 | -4 | 14 | 17 | 9 | 16 | -4 | 4 | 14 | 36 | 39 | 9 | -3 | -1 | 15 | 37 | 34 | 8 |
| 30 | 0 | 13 | 125 | 123 | 3 | 2 | 2 | 13 | 51 | 53 | 4 | -3 | -4 | 14 | 13 | 1 | 12 | -4 | 4 | 14 | 75 | 67 | 4 | -2 | -1 | 15 | 22 | 17 | 21 |
| 31 | 0 | 13 | 83 | 81 | 4 | 3 | 2 | 13 | 41 | 40 | 7 | -2 | -4 | 14 | 90 | 83 | 3 | -3 | 4 | 14 | 38 | 47 | 8 | -1 | -1 | 15 | 118 | 113 | 2 |
| 32 | 0 | 13 | 2 | 5 | 1 | 1 | 2 | 13 | 41 | 41 | 8 | -1 | -4 | 14 | 79 | 72 | 3 | -2 | 4 | 14 | 13 | 12 | 13 | 0 | -1 | 15 | 16 | 6 | 15 |
| 33 | 0 | 13 | 42 | 40 | 9 | 4 | 4 | 13 | 25 | 11 | 21 | 0 | -4 | 14 | 56 | 56 | 3 | -1 | 4 | 14 | 39 | 40 | 5 | 1 | -1 | 15 | 113 | 116 | 2 |
| 34 | 0 | 13 | 101 | 92 | 3 | 5 | 5 | 13 | 35 | 29 | 11 | 1 | -4 | 14 | 43 | 45 | 5 | 0 | 4 | 14 | 35 | 39 | 6 | 2 | -1 | 15 | 7 | 21 | 7 |
| 35 | 0 | 13 | 23 | 28 | 23 | -6 | 5 | 13 | 16 | 18 | 15 | 2 | -4 | 14 | 58 | 55 | 5 | 2 | 4 | 14 | 7 | 10 | 6 | 3 | -1 | 15 | 0 | 17 | 1 |
| 36 | 0 | 13 | 137 | 134 | 2 | -5 | 5 | 13 | 0 | 6 | 1 | 5 | -4 | 14 | 0 | 1 | 1 | -5 | 4 | 14 | 24 | 26 | 24 | 4 | -1 | 15 | 0 | 13 | 1 |
| 37 | 0 | 13 | 168 | 174 | 2 | -4 | 3 | 13 | 31 | 36 | 10 | 4 | -4 | 14 | 93 | 93 | 4 | -5 | 4 | 14 | 0 | 13 | 1 | -6 | 0 | 15 | 27 | 26 | 19 |
| 38 | 0 | 13 | 34 | 32 | 6 | -3 | 3 | 13 | 29 | 23 | 11 | 5 | -4 | 14 | 76 | 70 | 5 | -5 | 5 | 14 | 0 | 8 | 1 | -5 | 0 | 15 | 58 | 47 | 5 |
| 39 | 0 | 13 | 40 | 40 | 8 | -2 | 3 | 13 | 19 | 16 | 18 | -5 | -3 | 14 | 22 | 1 | 21 | -4 | 5 | 14 | 28 | 24 | 15 | -4 | 0 | 15 | 3 | 13 | 2 |
| 40 | 0 | 13 | 75 | 73 | 4 | -1 | 0 | 13 | 48 | 47 | 4 | -4 | -3 | 14 | 59 | 50 | 5 | -3 | 5 | 14 | 38 | 41 | 9 | -3 | 0 | 15 | 124 | 113 | 3 |
| 41 | 0 | 13 | 16 | 7 | 16 | 0 | 3 | 13 | 49 | 47 | 4 | -3 | -3 | 14 | 10 | 5 | 9 | -1 | 5 | 14 | 7 | 21 | 6 | -2 | 0 | 15 | 32 | 22 | 11 |
| 42 | 0 | 13 | 66 | 62 | 5 | 1 | 1 | 13 | 54 | 57 | 3 | -2 | -3 | 14 | 39 | 37 | 8 | 0 | 5 | 14 | 76 | 76 | 3 | -1 | 0 | 15 | 67 | 62 | 3 |
| 43 | 0 | 13 | 33 | 32 | 13 | 3 | 3 | 13 | 45 | 51 | 7 | -1 | -3 | 14 | 65 | 62 | 3 | -1 | 5 | 14 | 59 | 51 | 4 | 0 | 0 | 15 | 0 | 18 | 1 |
| 44 | 0 | 13 | 0 | 5 | 1 | 2 | 2 | 13 | 54 | 49 | 6 | 0 | -3 | 14 | 114 | 110 | 2 | -3 | 5 | 14 | 47 | 41 | 7 | 1 | 0 | 15 | 26 | 28 | 8 |
| 45 | 0 | 13 | 25 | 27 | 21 | 4 | 4 | 13 | 0 | 7 | 1 | 1 | -3 | 14 | 33 | 41 | 6 | -5 | 6 | 14 | 37 | 35 | 11 | 3 | 0 | 15 | 0 | 5 | 1 |
| 46 | 0 | 13 | 31 | 31 | 18 | -6 | 4 | 13 | 38 | 33 | 9 | 2 | -3 | 14 | 43 | 46 | 7 | -4 | 6 | 14 | 88 | 83 | 4 | 4 | 0 | 15 | 44 | 33 | 8 |
| 47 | 0 | 13 | 71 | 78 | 3 | -5 | 4 | 13 | 108 | 112 | 3 | -4 | -3 | 14 | 38 | 37 | 8 | -3 | 6 | 14 | 26 | 11 | 20 | -6 | 1 | 15 | 26 | 5 | 17 |
| 48 | 0 | 13 | 55 | 52 | 4 | -4 | 4 | 13 | 32 | 24 | 10 | 5 | -3 | 14 | 12 | 9 | 11 | -2 | 6 | 14 | 96 | 104 | 3 | -5 | 1 | 15 | 33 | 38 | 10 |
| 49 | 0 | 13 | 33 | 30 | 6 | -3 | 4 | 13 | 118 | 120 | 2 | -5 | -3 | 14 | 22 | 5 | 22 | 0 | 6 | 14 | 20 | 21 | 20 | -4 | 1 | 15 | 33 | 39 | 10 |
| 50 | 0 | 13 | 67 | 71 | 4 | -2 | 4 | 13 | 108 | 109 | 3 | -4 | -2 | 14 | 44 | 43 | 8 | -1 | 6 | 14 | 70 | 62 | 3 | -3 | 1 | 15 | 26 | 15 | 14 |
| 51 | 0 | 13 | 52 | 56 | 6 | -1 | 4 | 13 | 87 | 77 | 2 | -3 | -2 | 14 | 28 | 26 | 13 | -2 | 6 | 14 | 50 | 44 | 5 | -2 | 1 | 15 | 69 | 70 | 4 |
| 52 | 0 | 13 | 15 | 2 | 15 | 1 | 4 | 13 | 69 | 78 | 3 | -2 | -2 | 14 | 64 | 63 | 4 | 2 | 6 | 14 | 15 | 9 | 14 | -1 | 1 | 15 | 0 | 1 | 1 |
| 53 | 0 | 13 | 64 | 64 | 5 | 2 | 4 | 13 | 22 | 26 | 21 | -1 | -2 | 14 | 133 | 139 | 2 | -4 | 7 | 14 | 40 | 37 | 9 | 0 | 1 | 15 | 121 | 119 | 2 |
| 54 | 0 | 13 | 11 | 11 | 1 | 3 | 4 | 13 | 16 | 18 | 15 | 0 | -2 | 14 | 47 | 52 | 4 | -3 | 7 | 14 | 88 | 88 | 4 | 1 | 1 | 15 | 20 | 24 | 16 |
| 55 | 0 | 13 | 72 | 74 | 4 | -4 | 4 | 13 | 31 | 17 | 13 | 1 | -2 | 14 | 77 | 74 | 2 | -2 | 7 | 14 | 73 | 78 | 5 | 2 | 1 | 15 | 102 | 107 | 3 |
| 56 | 0 | 13 | 21 | 24 | 21 | -6 | 5 | 13 | 26 | 22 | 21 | 2 | -2 | 14 | 56 | 51 | 5 | -1 | 7 | 14 | 33 | 18 | 8 | 3 | 1 | 15 | 48 | 48 | 7 |
| 57 | 0 | 13 | 62 | 60 | 3 | -5 | 5 | 13 | 40 | 31 | 8 | 3 | -2 | 14 | 80 | 78 | 4 | 0 | 7 | 14 | 15 | 3 | 15 | | | | | | |

Table 1.

Observed and calculated structure factors for

1

| | | | 10Fo | | | 10Fc | | | 10s | | | | | | 10Fo | | | 10Fc | | | 10s | | | | | | 10Fo | | | 10Fc | | | 10s | | | | | | | | | | | | | | |
|----|---|----|------|----|----|------|----|----|-----|-----|----|----|----|----|------|-----|----|------|----|----|-----|----|----|----|----|----|------|-----|----|------|----|----|-----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l | h | k | l |
| 3 | 4 | 15 | 58 | 48 | 7 | 2 | -1 | 16 | 42 | 40 | 5 | -2 | -5 | 17 | 54 | 46 | 7 | -3 | 4 | 17 | 86 | 79 | 4 | -1 | 3 | 18 | 16 | 15 | 15 | | | | | | | | | | | | | | | | | | |
| -5 | 5 | 15 | 34 | 28 | 11 | -1 | -1 | 16 | 25 | 26 | 20 | -1 | -5 | 17 | 0 | 16 | 1 | -2 | 4 | 17 | 42 | 45 | 8 | 0 | 3 | 18 | 44 | 45 | 6 | 6 | 8 | | | | | | | | | | | | | | | | |
| -4 | 5 | 15 | 0 | 18 | 1 | 3 | -1 | 16 | 26 | 32 | 19 | 0 | -5 | 17 | 59 | 67 | 4 | -1 | 4 | 17 | 78 | 76 | 3 | -4 | 3 | 18 | 33 | 32 | 8 | 8 | 8 | | | | | | | | | | | | | | | | |
| -3 | 5 | 15 | 92 | 95 | 4 | -1 | -1 | 16 | 36 | 36 | 11 | 0 | -5 | 17 | 16 | 12 | 16 | 0 | 4 | 17 | 60 | 59 | 4 | -4 | 4 | 18 | 25 | 23 | 25 | 25 | 25 | | | | | | | | | | | | | | | | |
| -2 | 5 | 15 | 20 | 16 | 20 | -5 | 0 | 16 | 0 | 19 | 1 | 1 | -2 | -5 | 17 | 33 | 32 | 13 | 1 | 4 | 17 | 24 | 31 | 15 | -3 | 4 | 18 | 32 | 18 | 14 | 14 | 14 | | | | | | | | | | | | | | | |
| -1 | 5 | 15 | 94 | 96 | 2 | -3 | 0 | 16 | 25 | 17 | 17 | -3 | -4 | 17 | 0 | 0 | 1 | 2 | 4 | 17 | 28 | 27 | 19 | -2 | 4 | 18 | 16 | 5 | 15 | 15 | 15 | | | | | | | | | | | | | | | | |
| 0 | 5 | 15 | 56 | 54 | 7 | -3 | 0 | 16 | 55 | 57 | 5 | -2 | -4 | 17 | 0 | 23 | 7 | 1 | 1 | 17 | 35 | 32 | 11 | -1 | 4 | 18 | 0 | 11 | 1 | 1 | 1 | 1 | | | | | | | | | | | | | | | |
| 1 | 5 | 15 | 78 | 72 | 4 | -2 | 0 | 16 | 0 | 11 | 1 | -1 | -4 | 17 | 69 | 66 | 7 | -3 | 5 | 17 | 34 | 31 | 12 | 0 | 4 | 18 | 25 | 34 | 13 | 13 | 13 | | | | | | | | | | | | | | | | |
| 2 | 5 | 15 | 0 | 9 | 1 | 0 | 0 | 16 | 62 | 68 | 3 | 0 | -4 | 17 | 92 | 87 | 2 | -2 | 5 | 17 | 26 | 5 | 25 | 1 | 0 | 18 | 24 | 10 | 16 | 16 | 16 | | | | | | | | | | | | | | | | |
| 3 | 5 | 15 | 47 | 44 | 8 | -1 | 0 | 16 | 10 | 8 | 10 | 0 | -4 | 17 | 25 | 17 | 12 | -1 | 5 | 17 | 29 | 28 | 10 | -3 | 5 | 18 | 30 | 31 | 16 | 16 | 16 | | | | | | | | | | | | | | | | |
| 4 | 5 | 15 | 71 | 71 | 5 | 1 | 0 | 16 | 93 | 84 | 2 | 2 | -4 | 17 | 29 | 27 | 16 | 0 | 0 | 17 | 40 | 35 | 7 | -2 | 5 | 18 | 63 | 65 | 6 | 6 | 6 | | | | | | | | | | | | | | | | |
| 5 | 5 | 15 | 25 | 37 | 25 | 3 | 0 | 16 | 70 | 71 | 4 | 4 | -3 | 17 | 22 | 6 | 21 | 1 | 1 | 17 | 31 | 33 | 10 | -1 | 5 | 18 | 24 | 22 | 16 | 16 | 16 | | | | | | | | | | | | | | | | |
| 6 | 5 | 15 | 55 | 46 | 6 | 3 | 0 | 16 | 50 | 48 | 7 | -4 | -3 | 17 | 0 | 8 | 1 | -3 | 6 | 17 | 21 | 26 | 20 | 0 | 0 | 18 | 50 | 55 | 6 | 6 | 6 | | | | | | | | | | | | | | | | |
| 7 | 5 | 15 | 34 | 30 | 11 | 4 | 0 | 16 | 25 | 28 | 24 | -3 | -3 | 17 | 0 | 1 | 1 | -2 | 6 | 17 | 75 | 80 | 4 | 0 | 0 | 19 | 0 | 4 | 1 | 1 | 1 | 1 | | | | | | | | | | | | | | | |
| 8 | 5 | 15 | 21 | 26 | 20 | -5 | 1 | 16 | 25 | 18 | 24 | -2 | -3 | 17 | 0 | 5 | 5 | -1 | 6 | 17 | 75 | 80 | 4 | 0 | 0 | 19 | 59 | 63 | 4 | 4 | 4 | 4 | | | | | | | | | | | | | | | |
| 9 | 5 | 15 | 0 | 8 | 1 | -4 | 1 | 16 | 43 | 37 | 7 | -1 | -3 | 17 | 98 | 94 | 2 | -2 | 5 | 18 | 16 | 18 | 16 | -2 | -4 | 19 | 0 | 1 | 1 | 1 | 1 | 1 | | | | | | | | | | | | | | | |
| 10 | 5 | 15 | 0 | 5 | 1 | -3 | 1 | 16 | 38 | 26 | 8 | 0 | 0 | 17 | 0 | 17 | 1 | -1 | 5 | 18 | 16 | 12 | 13 | -2 | -3 | 19 | 16 | 15 | 16 | 16 | 16 | | | | | | | | | | | | | | | | |
| 11 | 5 | 15 | 27 | 20 | 26 | -2 | 1 | 16 | 21 | 16 | 20 | -2 | 1 | -3 | 17 | 56 | 53 | 4 | -1 | 5 | 18 | 0 | 8 | 1 | -1 | 0 | 19 | 19 | 2 | 18 | 18 | 18 | | | | | | | | | | | | | | | |
| 12 | 5 | 15 | 0 | 4 | 1 | -1 | 1 | 16 | 85 | 88 | 2 | 2 | -3 | 17 | 78 | 80 | 4 | 0 | 0 | 18 | 52 | 54 | 5 | 5 | 6 | 20 | 25 | 6 | 6 | 6 | 6 | 6 | | | | | | | | | | | | | | | |
| 13 | 5 | 15 | 26 | 29 | 26 | 0 | 0 | 16 | 81 | 82 | 2 | 2 | -3 | 17 | 19 | 2 | 18 | 1 | -5 | 18 | 43 | 48 | 6 | 5 | 6 | 21 | 50 | 47 | 8 | 8 | 8 | 8 | | | | | | | | | | | | | | | |
| 14 | 5 | 15 | 29 | 27 | 10 | -1 | 1 | 16 | 24 | 30 | 10 | -4 | -2 | 17 | 30 | 27 | 15 | -3 | -4 | 18 | 77 | 64 | 5 | -3 | -2 | 19 | 0 | 6 | 1 | 1 | 1 | 1 | | | | | | | | | | | | | | | |
| 15 | 5 | 15 | 12 | 2 | 11 | 3 | 1 | 16 | 80 | 67 | 4 | -3 | -2 | 17 | 79 | 84 | 4 | -2 | -4 | 18 | 42 | 42 | 10 | -2 | -2 | 19 | 71 | 66 | 8 | 8 | 8 | 8 | | | | | | | | | | | | | | | |
| 16 | 5 | 15 | 20 | 10 | 20 | 2 | 2 | 16 | 46 | 34 | 8 | -2 | -2 | 17 | 52 | 49 | 6 | -1 | -4 | 18 | 85 | 81 | 3 | -1 | -2 | 19 | 39 | 31 | 5 | 5 | 5 | 5 | | | | | | | | | | | | | | | |
| 17 | 5 | 15 | 32 | 38 | 10 | -4 | 4 | 16 | 42 | 51 | 8 | -1 | 0 | -2 | 17 | 75 | 74 | 3 | 0 | -4 | 18 | 36 | 26 | 7 | 0 | -2 | 19 | 16 | 8 | 16 | 16 | 16 | | | | | | | | | | | | | | | |
| 18 | 5 | 15 | 22 | 18 | 22 | -5 | 2 | 16 | 49 | 51 | 6 | -2 | 1 | -2 | 17 | 82 | 85 | 2 | -2 | 4 | 18 | 32 | 37 | 9 | -3 | -1 | 19 | 42 | 46 | 9 | 9 | 9 | | | | | | | | | | | | | | | |
| 19 | 5 | 15 | 80 | 94 | 5 | -3 | 2 | 16 | 65 | 63 | 5 | 2 | 2 | -2 | 17 | 43 | 38 | 5 | -2 | 3 | 18 | 88 | 83 | 4 | -2 | -1 | 19 | 13 | 19 | 13 | 13 | 13 | | | | | | | | | | | | | | | |
| 20 | 5 | 15 | 63 | 61 | 6 | -3 | 2 | 16 | 0 | 6 | 6 | -3 | -2 | 17 | 75 | 73 | 5 | -2 | 3 | 18 | 0 | 20 | 1 | -3 | -1 | 19 | 42 | 46 | 9 | 9 | 9 | | | | | | | | | | | | | | | | |
| 21 | 5 | 15 | 60 | 56 | 4 | -3 | 2 | 16 | 49 | 47 | 4 | -5 | -1 | 17 | 29 | 24 | 15 | -1 | -3 | 18 | 14 | 7 | 14 | 0 | -1 | 19 | 101 | 100 | 2 | 2 | 2 | 2 | | | | | | | | | | | | | | | |
| 22 | 5 | 15 | 0 | 11 | 1 | -1 | 2 | 16 | 67 | 75 | 3 | -4 | -1 | 17 | 30 | 16 | 14 | 0 | 0 | 18 | 68 | 66 | 3 | 0 | -1 | 19 | 33 | 35 | 8 | 8 | 8 | 8 | | | | | | | | | | | | | | | |
| 23 | 5 | 15 | 12 | 15 | 11 | 0 | 1 | 16 | 25 | 33 | 10 | -3 | -1 | 17 | 135 | 132 | 3 | -2 | 1 | 17 | 0 | 6 | 1 | -1 | 1 | 19 | 43 | 45 | 6 | 6 | 6 | 6 | | | | | | | | | | | | | | | |
| 24 | 5 | 15 | 35 | 37 | 13 | 1 | 2 | 16 | 0 | 6 | 1 | -2 | -1 | 17 | 90 | 99 | 3 | -4 | -3 | 18 | 57 | 55 | 6 | -3 | 0 | 19 | 18 | 39 | 10 | 10 | 10 | 10 | | | | | | | | | | | | | | | |
| 25 | 5 | 15 | 0 | 9 | 1 | 2 | 2 | 16 | 0 | 25 | 1 | -1 | -1 | 17 | 25 | 32 | 11 | -4 | -2 | 18 | 25 | 24 | 25 | -3 | 0 | 19 | 40 | 41 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | |
| 26 | 5 | 15 | 34 | 32 | 14 | -3 | 3 | 16 | 68 | 66 | 5 | 0 | -1 | 17 | 21 | 14 | 18 | -3 | -2 | 18 | 30 | 21 | 15 | -2 | 0 | 19 | 40 | 41 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | |
| 27 | 5 | 15 | 74 | 73 | 5 | -5 | 3 | 16 | 0 | 0 | 4 | -4 | 1 | -1 | 17 | 43 | 48 | 5 | -2 | 1 | 18 | 36 | 28 | 10 | -1 | 0 | 19 | 19 | 18 | 18 | 18 | 18 | | | | | | | | | | | | | | | |
| 28 | 5 | 15 | 31 | 26 | 8 | -4 | 4 | 16 | 36 | 35 | 9 | -2 | 2 | -1 | 17 | 8 | 11 | 8 | -2 | 2 | 18 | 30 | 41 | 9 | 0 | 0 | 19 | 16 | 8 | 15 | 15 | 15 | | | | | | | | | | | | | | | |
| 29 | 5 | 15 | 92 | 80 | 2 | -3 | 3 | 16 | 0 | 4 | 1 | 3 | -1 | 17 | 71 | 70 | 5 | -2 | 1 | 18 | 82 | 86 | 3 | 0 | 0 | 19 | 60 | 57 | 4 | 4 | 4 | 4 | | | | | | | | | | | | | | | |
| 30 | 5 | 15 | 70 | 71 | 3 | -2 | 3 | 16 | 8 | 8 | 1 | -5 | 0 | 17 | 46 | 44 | 8 | 0 | 0 | 17 | 73 | 70 | 3 | 2 | 2 | 19 | 48 | 29 | 8 | 8 | 8 | 8 | | | | | | | | | | | | | | | |
| 31 | 5 | 15 | 89 | 96 | 4 | -1 | 0 | 16 | 50 | 51 | 4 | -4 | 0 | 17 | 0 | 1 | 1 | 5 | 2 | 18 | 0 | 18 | 1 | -3 | 1 | 19 | 17 | 8 | 16 | 16 | 16 | 16 | | | | | | | | | | | | | | | |
| 32 | 5 | 15 | 0 | 16 | 1 | 0 | 3 | 16 | 34 | 30 | 7 | -3 | 0 | 17 | 59 | 60 | 10 | -4 | -2 | 18 | 56 | 56 | 6 | -1 | 1 | 19 | 27 | 23 | 17 | 17 | 17 | 17 | | | | | | | | | | | | | | | |
| 33 | 5 | 15 | 15 | 10 | 15 | 2 | 2 | 16 | 23 | 32 | 23 | -2 | 0 | 17 | 11 | 16 | 10 | -4 | -1 | 18 | 56 | 56 | 6 | -1 | 1 | 19 | 43 | 41 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | |
| 34 | 5 | 15 | 32 | 34 | 13 | -5 | 3 | 16 | 12 | 9 | 12 | -1 | 0 | 17 | 79 | 76 | 3 | -3 | -1 | 18 | 0 | 3 | 1 | 1 | 1 | 19 | 48 | 47 | 5 | 5 | 5 | 5 | | | | | | | | | | | | | | | |
| 35 | 5 | 15 | 30 | 36 | 9 | -4 | 4 | 16 | 8 | 7 | 8 | 0 | 0 | 17 | 33 | 28 | 5 | -1 | 1 | 18 | 21 | 2 | 20 | -3 | 2 | 19 | 52 | 46 | 7 | 7 | 7 | 7 | | | | | | | | | | | | | | | |
| 36 | 5 | 15 | 82 | 85 | 5 | -4 | 4 | 16 | 79 | 76 | 4 | 2 | 2 | 0 | 17 | 18 | 12 | 17 | 0 | 0 | 18 | 69 | 64 | 3 | -3 | 2 | 19 | 43 | 35 | 8 | 8 | 8 | 8 | | | | | | | | | | | | | | |
| 37 | 5 | 15 | 45 | 54 | 5 | -3 | 4 | 16 | 31 | 23 | 12 | 2 | 0 | 17 | 53 | 49 | 7 | 3 | 0 | 17 | 53 | 49 | 7 | -1 | 1 | 18 | 32 | 40 | 8 | 8 | 8 | 8 | | | | | | | | | | | | | | | |
| 38 | 5 | 15 | 0 | 9 | 1 | -2 | 4 | 16 | 56 | 51 | 2 | -5 | 1 | 17 | 51 | 56 | 7 | 2 | 2 | 18 | 101 | 94 | 3 | 0 | 0 | 19 | 18 | 13 | 18 | 18 | 18 | 18 | | | | | | | | | | | | | | | |
| 39 | 5 | 15 | 99 | 99 | 4 | -2 | 4 | 16 | 123 | 110 | 4 | -4 | 1 | 17 | 34 | 29 | 11 | -4 | 0 | 18 | 75 | 70 | 5 | -3 | 3 | 19 | 41 | 35 | 10 | 10 | 10 | 10 | | | | | | | | | | | | | | | |
| 40 | 5 | 15 | 14 | 12 | 13 | 0 | 0 | 16 | 46 | 43 | 5 | -3 | 1 | 17 | 0 | 14 | 1 | -4 | 0 | 18 | 0 | 26 | 21 | -2 | 3 | 19 | 41 | 0 | 9 | 1 | 1 | 1 | 1 | | | | | | | | | | | | | | |
| 41 | 5 | 15 | 48 | 49 | 6 | -5 | 4 | 16 | 62 | 60 | 6 | -2 | 1 | 17 | 48 | 47 | 6 | -3 | 0 | 18 | 21 | 26 | 21 | -1 | 3 | 19 | 23 | 17 | 16 | 16 | 16 | 16 | | | | | | | | | | | | | | | |
| 42 | 5 | 15 | 0 | 4 | 1 | -4 | 5 | 16 | 44 | 34 | 8 | -1 | 1 | 17 | 37 | 33 | 6 | -2 | 0 | 18 | 21 | 26 | 21 | -1 | 3 | 19 | 45 | 45 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | |
| 43 | 5 | 15 | 38 | 38 | 7 | -3 | 5 | 16 | 67 | 66 | 5 | 1 | 1 | 17 | 69 | 75 | 3 | 0 | 0 | 18 | 15 | 17 | 14 | 0 | 0 | 19 | 41 | 41 | 7 | 7 | 7 | 7 | | | | | | | | | | | | | | | |
| 44 | 5 | 15 | 37 | 33 | 6 | -3 | 5 | 16 | 22 | 31 | 21 | 2 | 2 | 17 | 39 | 35 | 3 | 2 | 0 | 18 | 24 | 9 | 1 | -1 | 4 | 19 | 41 | 41 | 7 | 7 | 7 | 7 | | | | | | | | | | | | | | | |
| 45 | 5 | 15 | 43 | 43 | 5 | -2 | 5 | 16 | 75 | 73 | 6 | 3 | 1 | 17 | 7 | 7 | 7 | 3 | 0 | 18 | 52 | 55 | 7 | -2 | 2 | 19 | 0 | 2 | 1 | 1 | 1 | 1 | 1 | | | | | | | | | | | | | | |
| 46 | 5 | 15 | 73 | 69 | 5 | 0 | 0 | 16 | 36 | 40 | 7 | -5 | 2 | 17 | 14 | 10 | 14 | -4 | 1 | 18 | 29 | 19 | 14 | 0 | 0 | 19 | 33 | 34 | 9 | 9 | 9 | 9 | | | | | | | | | | | | | | | |
| 47 | 5 | 15 | 23 | 23 | 15 | -2 | 5 | 16 | 47 | 33 | 5 | -4 | 2 | 17 | 22 | 28 | 21 | -2 | 1 | 18 | 0 | 19 | 11 | -1 | -2 | 20 | 22 | | | | | | | | | | | | | | | | | | | | |