

# CHEMISTRY OF MATERIALS

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Table 1. Crystal data and structure refinement for 1.

|                                      |                                                                                                                            |
|--------------------------------------|----------------------------------------------------------------------------------------------------------------------------|
| Identification code                  | dh6021                                                                                                                     |
| Empirical formula                    | $C_{12}H_{10}CuMoN_2O_4$                                                                                                   |
| Formula weight                       | 405.70                                                                                                                     |
| Temperature                          | 293(2) K                                                                                                                   |
| Wavelength                           | 0.71073 Å                                                                                                                  |
| Crystal system                       | Orthrhombic                                                                                                                |
| Space group                          | Pbcn                                                                                                                       |
| Unit cell dimensions                 | $a = 22.04620(10)$ Å $\alpha = 90^\circ$<br>$b = 12.2957(2)$ Å $\beta = 90^\circ$<br>$c = 9.7560(2)$ Å $\gamma = 90^\circ$ |
| Volume, Z                            | $2644.59(7)$ Å <sup>3</sup> , 8                                                                                            |
| Density (calculated)                 | $2.038$ Mg/m <sup>3</sup>                                                                                                  |
| Absorption coefficient               | $2.569$ mm <sup>-1</sup>                                                                                                   |
| F(000)                               | 1592                                                                                                                       |
| Crystal size                         | 0.24 x 0.22 x 0.20 mm                                                                                                      |
| $\theta$ range for data collection   | 1.85 to $28.24^\circ$                                                                                                      |
| Limiting indices                     | $-28 \leq h \leq 29$ , $-16 \leq k \leq 9$ , $-12 \leq l \leq 12$                                                          |
| Reflections collected                | 15372                                                                                                                      |
| Independent reflections              | 3202 ( $R_{int} = 0.0617$ )                                                                                                |
| Refinement method                    | Full-matrix least-squares on $F^2$                                                                                         |
| Data / restraints / parameters       | 3202 / 0 / 221                                                                                                             |
| Goodness-of-fit on $F^2$             | 1.245                                                                                                                      |
| Final R indices [ $I > 2\sigma(I)$ ] | $R1 = 0.0558$ , $wR2 = 0.0824$                                                                                             |
| R indices (all data)                 | $R1 = 0.0643$ , $wR2 = 0.0877$                                                                                             |
| Largest diff. peak and hole          | 0.808 and $-0.663$ eÅ <sup>-3</sup>                                                                                        |

Table 2. Atomic coordinates [ $\times 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for 1.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

|       | x       | y        | z        | $U(\text{eq})$ |
|-------|---------|----------|----------|----------------|
| Mo(1) | 6956(1) | 6764(1)  | 266(1)   | 12(1)          |
| Cu(1) | 7539(1) | 9308(1)  | -1373(1) | 15(1)          |
| O(1)  | 7106(1) | 8100(3)  | -278(4)  | 18(1)          |
| O(2)  | 7321(2) | 5833(3)  | -852(4)  | 27(1)          |
| O(3)  | 7214(2) | 6593(3)  | 1960(4)  | 24(1)          |
| O(4)  | 6177(2) | 6534(3)  | 242(4)   | 22(1)          |
| N(1)  | 6763(2) | 9719(3)  | -2296(5) | 18(1)          |
| N(2)  | 8317(2) | 8935(3)  | -437(4)  | 15(1)          |
| C(1)  | 6557(2) | 10722(4) | -2470(6) | 19(1)          |
| C(2)  | 6036(2) | 10953(5) | -3225(6) | 21(1)          |
| C(3)  | 5707(2) | 10119(4) | -3834(6) | 19(1)          |
| C(4)  | 5921(3) | 9066(5)  | -3622(8) | 36(2)          |
| C(5)  | 6440(3) | 8909(5)  | -2868(8) | 36(2)          |
| C(6)  | 8856(2) | 8862(4)  | -1083(5) | 18(1)          |
| C(7)  | 9401(2) | 8792(4)  | -370(6)  | 17(1)          |
| C(8)  | 9399(2) | 8808(4)  | 1063(5)  | 13(1)          |
| C(9)  | 8838(2) | 8868(4)  | 1718(5)  | 14(1)          |
| C(10) | 8316(2) | 8929(4)  | 948(5)   | 15(1)          |
| C(11) | 5172(2) | 10354(5) | -4678(6) | 24(1)          |
| C(12) | 9978(2) | 8775(4)  | 1817(5)  | 16(1)          |

Table 3. Bond lengths [Å] and angles [°] for 1.

|                    |           |                     |           |
|--------------------|-----------|---------------------|-----------|
| Mo(1)-O(4)         | 1.740(3)  | Mo(1)-O(1)          | 1.758(3)  |
| Mo(1)-O(3)         | 1.760(4)  | Mo(1)-O(2)          | 1.775(4)  |
| Cu(1)-O(2)#1       | 1.967(4)  | Cu(1)-N(2)          | 1.996(4)  |
| Cu(1)-N(1)         | 1.999(4)  | Cu(1)-O(3)#2        | 2.042(4)  |
| Cu(1)-O(1)         | 2.064(3)  | O(2)-Cu(1)#3        | 1.967(4)  |
| O(3)-Cu(1)#4       | 2.042(4)  | N(1)-C(1)           | 1.325(7)  |
| N(1)-C(5)          | 1.346(7)  | N(2)-C(6)           | 1.347(6)  |
| N(2)-C(10)         | 1.351(6)  | C(1)-C(2)           | 1.394(7)  |
| C(2)-C(3)          | 1.389(7)  | C(3)-C(4)           | 1.392(8)  |
| C(3)-C(11)         | 1.468(7)  | C(4)-C(5)           | 1.374(8)  |
| C(6)-C(7)          | 1.393(7)  | C(7)-C(8)           | 1.398(7)  |
| C(8)-C(9)          | 1.394(7)  | C(8)-C(12)          | 1.475(6)  |
| C(9)-C(10)         | 1.377(7)  | C(11)-C(11)#5       | 1.315(11) |
| C(12)-C(12)#6      | 1.336(10) |                     |           |
| O(4)-Mo(1)-O(1)    | 109.5(2)  | O(4)-Mo(1)-O(3)     | 108.2(2)  |
| O(1)-Mo(1)-O(3)    | 109.5(2)  | O(4)-Mo(1)-O(2)     | 109.6(2)  |
| O(1)-Mo(1)-O(2)    | 109.3(2)  | O(3)-Mo(1)-O(2)     | 110.7(2)  |
| O(2)#1-Cu(1)-N(2)  | 88.1(2)   | O(2)#1-Cu(1)-N(1)   | 90.5(2)   |
| N(2)-Cu(1)-N(1)    | 178.6(2)  | O(2)#1-Cu(1)-O(3)#2 | 133.0(2)  |
| N(2)-Cu(1)-O(3)#2  | 90.6(2)   | N(1)-Cu(1)-O(3)#2   | 90.3(2)   |
| O(2)#1-Cu(1)-O(1)  | 128.7(2)  | N(2)-Cu(1)-O(1)     | 89.8(2)   |
| N(1)-Cu(1)-O(1)    | 91.1(2)   | O(3)#2-Cu(1)-O(1)   | 98.3(2)   |
| Mo(1)-O(1)-Cu(1)   | 156.4(2)  | Mo(1)-O(2)-Cu(1)#3  | 147.6(2)  |
| Mo(1)-O(3)-Cu(1)#4 | 154.0(2)  | C(1)-N(1)-C(5)      | 117.0(4)  |
| C(1)-N(1)-Cu(1)    | 125.9(3)  | C(5)-N(1)-Cu(1)     | 116.9(4)  |
| C(6)-N(2)-C(10)    | 118.0(4)  | C(6)-N(2)-Cu(1)     | 123.9(3)  |
| C(10)-N(2)-Cu(1)   | 117.1(3)  | N(1)-C(1)-C(2)      | 122.7(5)  |
| C(3)-C(2)-C(1)     | 120.3(5)  | C(2)-C(3)-C(4)      | 116.6(5)  |
| C(2)-C(3)-C(11)    | 120.9(5)  | C(4)-C(3)-C(11)     | 122.6(5)  |
| C(5)-C(4)-C(3)     | 119.5(5)  | N(1)-C(5)-C(4)      | 123.9(5)  |
| N(2)-C(6)-C(7)     | 122.1(5)  | C(6)-C(7)-C(8)      | 119.7(5)  |
| C(9)-C(8)-C(7)     | 117.5(4)  | C(9)-C(8)-C(12)     | 122.8(4)  |
| C(7)-C(8)-C(12)    | 119.7(4)  | C(10)-C(9)-C(8)     | 119.6(5)  |
| N(2)-C(10)-C(9)    | 123.0(5)  | C(11)#5-C(11)-C(3)  | 126.9(7)  |
| C(12)#6-C(12)-C(8) | 124.0(6)  |                     |           |

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y+1/2,z    #2 -x+3/2,-y+3/2,z-1/2    #3 -x+3/2,y-1/2,z  
 #4 -x+3/2,-y+3/2,z+1/2    #5 -x+1,-y+2,-z-1    #6 -x+2,y,-z+1/2

Table 4. Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [ (ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12} ]$$

|       | U11   | U22   | U33   | U23   | U13    | U12   |
|-------|-------|-------|-------|-------|--------|-------|
| Mo(1) | 12(1) | 14(1) | 11(1) | 0(1)  | 3(1)   | -1(1) |
| Cu(1) | 12(1) | 14(1) | 19(1) | 0(1)  | -8(1)  | 1(1)  |
| O(1)  | 19(2) | 18(2) | 17(2) | 6(2)  | -1(1)  | -3(1) |
| O(2)  | 26(2) | 17(2) | 38(2) | -7(2) | 21(2)  | -2(2) |
| O(3)  | 21(2) | 33(2) | 17(2) | 10(2) | -1(2)  | 0(2)  |
| O(4)  | 18(2) | 22(2) | 26(2) | -3(2) | 2(2)   | -7(2) |
| N(1)  | 16(2) | 11(2) | 26(2) | 2(2)  | -9(2)  | -1(2) |
| N(2)  | 15(2) | 13(2) | 16(2) | 0(2)  | -6(2)  | 0(2)  |
| C(1)  | 18(2) | 14(2) | 26(3) | 4(2)  | -10(2) | -4(2) |
| C(2)  | 19(2) | 16(3) | 29(3) | 4(2)  | -9(2)  | -2(2) |
| C(3)  | 18(2) | 17(3) | 22(3) | 1(2)  | -7(2)  | 1(2)  |
| C(4)  | 34(3) | 16(3) | 58(4) | -4(3) | -33(3) | -2(2) |
| C(5)  | 35(3) | 15(3) | 59(5) | 4(3)  | -31(3) | 4(3)  |
| C(6)  | 17(2) | 19(3) | 17(3) | -1(2) | -6(2)  | -2(2) |
| C(7)  | 13(2) | 22(3) | 16(2) | 3(2)  | -2(2)  | -2(2) |
| C(8)  | 12(2) | 11(2) | 16(3) | 3(2)  | -3(2)  | 1(2)  |
| C(9)  | 13(2) | 15(2) | 14(3) | 0(2)  | -4(2)  | -1(2) |
| C(10) | 14(2) | 19(3) | 13(2) | -5(2) | -3(2)  | -2(2) |
| C(11) | 21(2) | 19(3) | 33(3) | 5(3)  | -13(2) | 5(2)  |
| C(12) | 11(2) | 19(3) | 17(3) | 0(2)  | -1(2)  | -1(2) |

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

|       | x         | y         | z         | U(eq)  |
|-------|-----------|-----------|-----------|--------|
| H(1)  | 6803(22)  | 11297(43) | -2114(52) | 11(13) |
| H(2)  | 5917(24)  | 11632(48) | -3343(56) | 19(15) |
| H(4)  | 5718(28)  | 8398(53)  | -3964(65) | 38(18) |
| H(5)  | 6593(28)  | 8287(55)  | -2687(64) | 34(17) |
| H(6)  | 8859(23)  | 8843(46)  | -2056(58) | 16(14) |
| H(7)  | 9735(26)  | 8774(46)  | -845(57)  | 20(15) |
| H(9)  | 8807(26)  | 8805(50)  | 2675(64)  | 27(17) |
| H(10) | 7942(22)  | 8993(40)  | 1364(50)  | 7(12)  |
| H(11) | 5094(28)  | 11034(51) | -4749(67) | 32(17) |
| H(12) | 10336(23) | 8753(42)  | 1290(52)  | 12(13) |

Table 1. Crystal data and structure refinement for 1.

|                                      |                                                                                                                                 |
|--------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| Identification code                  | dh6013                                                                                                                          |
| Empirical formula                    | $C_{12}H_{12}CuN_2O_5S$                                                                                                         |
| Formula weight                       | 359.84                                                                                                                          |
| Temperature                          | 293(2) K                                                                                                                        |
| Wavelength                           | 0.71073 Å                                                                                                                       |
| Crystal system                       | Monoclinic                                                                                                                      |
| Space group                          | Pn                                                                                                                              |
| Unit cell dimensions                 | $a = 7.2851(2)$ Å $\alpha = 90^\circ$<br>$b = 9.9062(3)$ Å $\beta = 98.2070(10)^\circ$<br>$c = 9.1407(2)$ Å $\gamma = 90^\circ$ |
| Volume, Z                            | $652.91(3)$ Å <sup>3</sup> , 2                                                                                                  |
| Density (calculated)                 | $1.830$ Mg/m <sup>3</sup>                                                                                                       |
| Absorption coefficient               | $1.856$ mm <sup>-1</sup>                                                                                                        |
| F(000)                               | 366                                                                                                                             |
| Crystal size                         | $0.35 \times 0.31 \times 0.31$ mm                                                                                               |
| $\theta$ range for data collection   | $2.06$ to $28.30^\circ$                                                                                                         |
| Limiting indices                     | $-5 \leq h \leq 9$ , $-13 \leq k \leq 13$ , $-11 \leq l \leq 12$                                                                |
| Reflections collected                | 4209                                                                                                                            |
| Independent reflections              | 1968 ( $R_{int} = 0.0363$ )                                                                                                     |
| Absorption correction                | Psi                                                                                                                             |
| Max. and min. transmission           | 0.543 and 0.865                                                                                                                 |
| Refinement method                    | Full-matrix least-squares on $F^2$                                                                                              |
| Data / restraints / parameters       | 1968 / 2 / 198                                                                                                                  |
| Goodness-of-fit on $F^2$             | 1.076                                                                                                                           |
| Final R indices [ $I > 2\sigma(I)$ ] | $R1 = 0.0274$ , $wR2 = 0.0733$                                                                                                  |
| R indices (all data)                 | $R1 = 0.0281$ , $wR2 = 0.0743$                                                                                                  |
| Absolute structure parameter         | 0.00                                                                                                                            |
| Largest diff. peak and hole          | $0.500$ and $-0.565$ eÅ <sup>-3</sup>                                                                                           |

Table 2. Atomic coordinates [ $\times 10^4$ ] and equivalent isotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for 1.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

|       | x       | y        | z        | $U(\text{eq})$ |
|-------|---------|----------|----------|----------------|
| Cu(1) | 9199(1) | 9772(1)  | 4663(1)  | 10(1)          |
| S(1)  | 7278(1) | 11466(1) | 2109(1)  | 11(1)          |
| O(1)  | 7079(4) | 10538(3) | 3362(3)  | 14(1)          |
| O(2)  | 6670(4) | 10748(3) | 684(3)   | 13(1)          |
| O(3)  | 9248(4) | 11816(3) | 2155(3)  | 17(1)          |
| O(4)  | 6110(4) | 12648(3) | 2216(3)  | 19(1)          |
| O(5)  | 7642(4) | 8466(3)  | 6145(3)  | 19(1)          |
| N(1)  | 9375(5) | 8216(3)  | 3217(4)  | 14(1)          |
| N(2)  | 9271(4) | 1412(3)  | -4001(3) | 13(1)          |
| C(1)  | 9297(6) | 6937(4)  | 3687(4)  | 19(1)          |
| C(2)  | 9358(6) | 5829(4)  | 2772(4)  | 19(1)          |
| C(3)  | 9553(6) | 6017(4)  | 1284(4)  | 15(1)          |
| C(4)  | 9698(6) | 7349(4)  | 807(4)   | 14(1)          |
| C(5)  | 9602(5) | 8407(4)  | 1789(4)  | 14(1)          |
| C(6)  | 9480(7) | 4828(4)  | 309(5)   | 18(1)          |
| C(7)  | 9628(7) | 4853(4)  | -1123(5) | 19(1)          |
| C(8)  | 9491(6) | 3656(4)  | -2083(4) | 15(1)          |
| C(9)  | 9037(5) | 2367(3)  | -1625(4) | 13(1)          |
| C(10) | 8950(5) | 1293(4)  | -2583(4) | 13(1)          |
| C(11) | 9711(6) | 2640(4)  | -4459(4) | 17(1)          |
| C(12) | 9841(6) | 3772(4)  | -3549(4) | 19(1)          |

Table 3. Bond lengths [Å] and angles [°] for 1.

|                     |            |                    |            |
|---------------------|------------|--------------------|------------|
| Cu(1)-O(1)          | 1.962(3)   | Cu(1)-O(2)#1       | 1.974(3)   |
| Cu(1)-N(2)#2        | 2.029(3)   | Cu(1)-N(1)         | 2.047(3)   |
| Cu(1)-O(5)          | 2.288(3)   | S(1)-O(4)          | 1.459(3)   |
| S(1)-O(3)           | 1.471(3)   | S(1)-O(1)          | 1.492(3)   |
| S(1)-O(2)           | 1.495(2)   | O(2)-Cu(1)#3       | 1.974(3)   |
| N(1)-C(1)           | 1.342(5)   | N(1)-C(5)          | 1.352(5)   |
| N(2)-C(11)          | 1.340(5)   | N(2)-C(10)         | 1.354(5)   |
| N(2)-Cu(1)#4        | 2.029(3)   | C(1)-C(2)          | 1.385(5)   |
| C(2)-C(3)           | 1.400(5)   | C(3)-C(4)          | 1.398(5)   |
| C(3)-C(6)           | 1.473(5)   | C(4)-C(5)          | 1.388(5)   |
| C(6)-C(7)           | 1.329(6)   | C(7)-C(8)          | 1.471(5)   |
| C(8)-C(9)           | 1.398(5)   | C(8)-C(12)         | 1.404(5)   |
| C(9)-C(10)          | 1.373(5)   | C(11)-C(12)        | 1.391(5)   |
| O(1)-Cu(1)-O(2)#1   | 166.67(11) | O(1)-Cu(1)-N(2)#2  | 90.33(12)  |
| O(2)#1-Cu(1)-N(2)#2 | 88.91(12)  | O(1)-Cu(1)-N(1)    | 90.93(12)  |
| O(2)#1-Cu(1)-N(1)   | 88.37(12)  | N(2)#2-Cu(1)-N(1)  | 173.44(14) |
| O(1)-Cu(1)-O(5)     | 99.43(12)  | O(2)#1-Cu(1)-O(5)  | 93.90(11)  |
| N(2)#2-Cu(1)-O(5)   | 93.94(12)  | N(1)-Cu(1)-O(5)    | 92.20(12)  |
| O(4)-S(1)-O(3)      | 112.7(2)   | O(4)-S(1)-O(1)     | 108.7(2)   |
| O(3)-S(1)-O(1)      | 108.9(2)   | O(4)-S(1)-O(2)     | 109.7(2)   |
| O(3)-S(1)-O(2)      | 107.7(2)   | O(1)-S(1)-O(2)     | 109.1(2)   |
| S(1)-O(1)-Cu(1)     | 123.3(2)   | S(1)-O(2)-Cu(1)#3  | 132.3(2)   |
| C(1)-N(1)-C(5)      | 117.3(3)   | C(1)-N(1)-Cu(1)    | 119.7(3)   |
| C(5)-N(1)-Cu(1)     | 123.1(2)   | C(11)-N(2)-C(10)   | 117.4(3)   |
| C(11)-N(2)-Cu(1)#4  | 121.7(3)   | C(10)-N(2)-Cu(1)#4 | 120.9(2)   |
| N(1)-C(1)-C(2)      | 123.2(4)   | C(1)-C(2)-C(3)     | 119.9(3)   |
| C(4)-C(3)-C(2)      | 116.8(3)   | C(4)-C(3)-C(6)     | 124.3(3)   |
| C(2)-C(3)-C(6)      | 118.8(3)   | C(5)-C(4)-C(3)     | 119.9(3)   |
| N(1)-C(5)-C(4)      | 122.9(3)   | C(7)-C(6)-C(3)     | 125.4(4)   |
| C(6)-C(7)-C(8)      | 124.4(4)   | C(9)-C(8)-C(12)    | 116.3(3)   |
| C(9)-C(8)-C(7)      | 123.9(3)   | C(12)-C(8)-C(7)    | 119.8(3)   |
| C(10)-C(9)-C(8)     | 120.5(3)   | N(2)-C(10)-C(9)    | 123.0(3)   |
| N(2)-C(11)-C(12)    | 122.9(3)   | C(11)-C(12)-C(8)   | 119.9(3)   |

Symmetry transformations used to generate equivalent atoms:

#1  $x+1/2, -y+2, z+1/2$     #2  $x, y+1, z+1$     #3  $x-1/2, -y+2, z-1/2$   
#4  $x, y-1, z-1$

Table 4. Anisotropic displacement parameters [ $\text{\AA}^2 \times 10^3$ ] for 1.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [ (ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12} ]$$

|       | U11   | U22   | U33   | U23   | U13  | U12   |
|-------|-------|-------|-------|-------|------|-------|
| Cu(1) | 12(1) | 10(1) | 9(1)  | -2(1) | 2(1) | 1(1)  |
| S(1)  | 12(1) | 10(1) | 10(1) | 0(1)  | 2(1) | 0(1)  |
| O(1)  | 14(1) | 17(1) | 11(1) | 2(1)  | 2(1) | 0(1)  |
| O(2)  | 13(1) | 16(1) | 10(1) | -2(1) | 1(1) | 0(1)  |
| O(3)  | 12(1) | 23(1) | 17(1) | -5(1) | 4(1) | -4(1) |
| O(4)  | 21(1) | 16(1) | 21(1) | -4(1) | 4(1) | 6(1)  |
| O(5)  | 14(1) | 23(2) | 21(1) | 3(1)  | 8(1) | -1(1) |
| N(1)  | 16(2) | 15(1) | 10(1) | 0(1)  | 3(1) | 0(1)  |
| N(2)  | 13(2) | 12(1) | 14(1) | -4(1) | 1(1) | 2(1)  |
| C(1)  | 29(2) | 16(2) | 12(2) | -3(1) | 4(2) | 3(2)  |
| C(2)  | 33(2) | 11(2) | 14(2) | -2(1) | 7(2) | 1(2)  |
| C(3)  | 20(2) | 13(2) | 11(2) | -3(1) | 3(1) | 1(1)  |
| C(4)  | 18(2) | 15(2) | 11(2) | -1(1) | 2(1) | 0(1)  |
| C(5)  | 16(2) | 13(2) | 13(2) | -1(1) | 4(1) | 1(1)  |
| C(6)  | 28(2) | 10(2) | 15(2) | -5(1) | 7(2) | -1(2) |
| C(7)  | 30(3) | 14(2) | 13(2) | -4(1) | 6(2) | -4(2) |
| C(8)  | 18(2) | 12(2) | 14(2) | -1(1) | 2(1) | 0(1)  |
| C(9)  | 15(2) | 14(2) | 9(2)  | -2(1) | 5(1) | -4(1) |
| C(10) | 14(2) | 10(2) | 15(2) | -1(1) | 2(1) | 1(1)  |
| C(11) | 23(2) | 16(2) | 12(2) | -5(1) | 3(2) | 2(2)  |
| C(12) | 31(2) | 11(2) | 14(2) | -2(1) | 6(2) | -5(2) |

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 1.

|        | x         | y        | z        | U(eq)  |
|--------|-----------|----------|----------|--------|
| H(1A)  | 9196(6)   | 6787(4)  | 4677(4)  | 22     |
| H(2A)  | 9270(6)   | 4961(4)  | 3145(4)  | 23     |
| H(4A)  | 9859(6)   | 7525(4)  | -165(4)  | 17     |
| H(5C)  | 9698(5)   | 9286(4)  | 1450(4)  | 17     |
| H(9A)  | 8792(5)   | 2235(3)  | -664(4)  | 15     |
| H(10A) | 8657(5)   | 446(4)   | -2243(4) | 16     |
| H(11A) | 9941(6)   | 2740(4)  | -5428(4) | 20     |
| H(12A) | 10159(6)  | 4604(4)  | -3911(4) | 22     |
| H(5B)  | 8368(67)  | 8078(44) | 6722(49) | 6(10)  |
| H(5A)  | 6699(125) | 8413(70) | 6476(75) | 62(23) |

Table 6. Observed and calculated structure factors for 1

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| 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  | 0 | 0 | 4984 | 5099 | 44  | 4  | 6  | 0 | 472  | 504  | 9   | 11 | 13 | 0 | 446  | 525  | 46  | 10 | 3 | 1 | 652  | 605  | 5   | 13 | 6 | 1 | 465  | 443  | 17  |
| 4  | 0 | 0 | 1534 | 1535 | 27  | 6  | 6  | 0 | 2026 | 2039 | 20  | 13 | 13 | 0 | 311  | 376  | 32  | 11 | 3 | 1 | 370  | 360  | 11  | 14 | 6 | 1 | 646  | 625  | 8   |
| 6  | 0 | 0 | 799  | 741  | 7   | 8  | 6  | 0 | 3211 | 3181 | 24  | 15 | 13 | 0 | 421  | 463  | 26  | 12 | 3 | 1 | 127  | 38   | 19  | 15 | 6 | 1 | 364  | 361  | 16  |
| 8  | 0 | 0 | 151  | 139  | 26  | 10 | 6  | 0 | 3096 | 3126 | 23  | 17 | 13 | 0 | 127  | 30   | 126 | 13 | 3 | 1 | 205  | 201  | 11  | 16 | 6 | 1 | 717  | 703  | 10  |
| 10 | 0 | 0 | 954  | 972  | 16  | 12 | 6  | 0 | 2498 | 2480 | 19  | 0  | 14 | 0 | 881  | 889  | 17  | 14 | 3 | 1 | 327  | 315  | 10  | 17 | 6 | 1 | 11   | 48   | 11  |
| 12 | 0 | 0 | 571  | 515  | 24  | 14 | 6  | 0 | 1209 | 1175 | 28  | 2  | 14 | 0 | 166  | 84   | 38  | 15 | 3 | 1 | 556  | 537  | 7   | 18 | 6 | 1 | 167  | 129  | 48  |
| 14 | 0 | 0 | 1310 | 1372 | 14  | 16 | 6  | 0 | 313  | 330  | 16  | 4  | 14 | 0 | 645  | 642  | 15  | 16 | 3 | 1 | 211  | 206  | 17  | 19 | 6 | 1 | 166  | 60   | 44  |
| 16 | 0 | 0 | 2343 | 2364 | 22  | 18 | 6  | 0 | 621  | 588  | 16  | 6  | 14 | 0 | 1324 | 1342 | 16  | 17 | 3 | 1 | 135  | 142  | 22  | 20 | 6 | 1 | 275  | 323  | 20  |
| 18 | 0 | 0 | 1302 | 1283 | 19  | 20 | 6  | 0 | 144  | 43   | 55  | 8  | 14 | 0 | 1564 | 1564 | 15  | 18 | 3 | 1 | 129  | 77   | 31  | 21 | 6 | 1 | 164  | 162  | 38  |
| 20 | 0 | 0 | 1741 | 1728 | 18  | 22 | 6  | 0 | 168  | 161  | 103 | 10 | 14 | 0 | 1618 | 1617 | 19  | 19 | 3 | 1 | 185  | 139  | 16  | 22 | 6 | 1 | 185  | 159  | 28  |
| 22 | 0 | 0 | 1531 | 1521 | 14  | 24 | 6  | 0 | 729  | 714  | 18  | 12 | 14 | 0 | 979  | 995  | 18  | 20 | 3 | 1 | 59   | 27   | 58  | 23 | 6 | 1 | 247  | 242  | 24  |
| 24 | 0 | 0 | 232  | 192  | 73  | 26 | 6  | 0 | 1115 | 1126 | 18  | 1  | 15 | 0 | 289  | 55   | 48  | 21 | 3 | 1 | 194  | 158  | 24  | 24 | 6 | 1 | 293  | 307  | 46  |
| 26 | 0 | 0 | 340  | 299  | 20  | 1  | 7  | 0 | 773  | 728  | 8   | 3  | 15 | 0 | 612  | 695  | 16  | 22 | 3 | 1 | 339  | 313  | 11  | 25 | 6 | 1 | 392  | 417  | 39  |
| 28 | 0 | 0 | 364  | 385  | 36  | 3  | 7  | 0 | 360  | 306  | 19  | 5  | 15 | 0 | 525  | 569  | 21  | 23 | 3 | 1 | 516  | 525  | 16  | 26 | 6 | 1 | 255  | 178  | 44  |
| 1  | 1 | 0 | 614  | 573  | 5   | 5  | 7  | 0 | 267  | 201  | 15  | 7  | 15 | 0 | 246  | 329  | 100 | 24 | 3 | 1 | 336  | 342  | 20  | 27 | 6 | 1 | 531  | 421  | 145 |
| 3  | 1 | 0 | 1356 | 1357 | 13  | 7  | 7  | 0 | 274  | 276  | 15  | 9  | 15 | 0 | 229  | 160  | 82  | 25 | 3 | 1 | 318  | 283  | 14  | 1  | 7 | 1 | 490  | 472  | 9   |
| 5  | 1 | 0 | 1609 | 1631 | 12  | 9  | 7  | 0 | 222  | 168  | 33  | 0  | 16 | 0 | 669  | 714  | 29  | 26 | 3 | 1 | 412  | 385  | 17  | 2  | 7 | 1 | 2362 | 2377 | 12  |
| 7  | 1 | 0 | 1305 | 1325 | 10  | 11 | 7  | 0 | 357  | 313  | 14  | 2  | 16 | 0 | 482  | 577  | 36  | 27 | 3 | 1 | 269  | 264  | 37  | 3  | 7 | 1 | 74   | 128  | 73  |
| 9  | 1 | 0 | 1153 | 1125 | 9   | 13 | 7  | 0 | 696  | 677  | 11  | 4  | 16 | 0 | 579  | 598  | 63  | 28 | 3 | 1 | 340  | 348  | 47  | 4  | 7 | 1 | 1872 | 1923 | 12  |
| 11 | 1 | 0 | 736  | 676  | 8   | 15 | 7  | 0 | 559  | 570  | 12  | 6  | 16 | 0 | 226  | 239  | 47  | 0  | 4 | 1 | 192  | 186  | 65  | 5  | 7 | 1 | 349  | 356  | 13  |
| 13 | 1 | 0 | 639  | 618  | 8   | 17 | 7  | 0 | 390  | 421  | 20  | 1  | 1  | 1 | 270  | 253  | 3   | 1  | 4 | 1 | 3348 | 3437 | 17  | 6  | 7 | 1 | 1849 | 1848 | 10  |
| 15 | 1 | 0 | 221  | 198  | 18  | 19 | 7  | 0 | 866  | 882  | 22  | 2  | 1  | 1 | 1262 | 1262 | 9   | 2  | 4 | 1 | 667  | 673  | 6   | 7  | 7 | 1 | 253  | 256  | 13  |
| 17 | 1 | 0 | 1152 | 1135 | 9   | 21 | 7  | 0 | 345  | 426  | 45  | 3  | 1  | 1 | 674  | 663  | 4   | 3  | 4 | 1 | 1374 | 1445 | 9   | 8  | 7 | 1 | 580  | 575  | 11  |
| 19 | 1 | 0 | 389  | 378  | 10  | 23 | 7  | 0 | 366  | 251  | 83  | 4  | 1  | 1 | 2996 | 3046 | 15  | 4  | 4 | 1 | 978  | 964  | 7   | 9  | 7 | 1 | 372  | 346  | 17  |
| 21 | 1 | 0 | 687  | 674  | 12  | 25 | 7  | 0 | 190  | 245  | 48  | 5  | 1  | 1 | 403  | 382  | 4   | 5  | 4 | 1 | 313  | 311  | 14  | 10 | 7 | 1 | 566  | 560  | 8   |
| 23 | 1 | 0 | 870  | 865  | 9   | 0  | 8  | 0 | 2008 | 2071 | 19  | 6  | 1  | 1 | 2218 | 2282 | 9   | 6  | 4 | 1 | 1237 | 1229 | 6   | 11 | 7 | 1 | 215  | 185  | 15  |
| 25 | 1 | 0 | 1033 | 1044 | 11  | 2  | 8  | 0 | 3192 | 3251 | 24  | 7  | 1  | 1 | 766  | 743  | 5   | 7  | 4 | 1 | 723  | 713  | 5   | 12 | 7 | 1 | 1397 | 1389 | 9   |
| 27 | 1 | 0 | 475  | 474  | 14  | 4  | 8  | 0 | 2076 | 2097 | 16  | 8  | 1  | 1 | 1693 | 1700 | 8   | 8  | 4 | 1 | 1211 | 1237 | 8   | 13 | 7 | 1 | 146  | 185  | 33  |
| 0  | 2 | 0 | 1369 | 1341 | 18  | 6  | 8  | 0 | 608  | 585  | 11  | 9  | 1  | 1 | 427  | 388  | 4   | 9  | 4 | 1 | 756  | 760  | 6   | 14 | 7 | 1 | 1514 | 1499 | 15  |
| 2  | 2 | 0 | 552  | 540  | 11  | 8  | 8  | 0 | 153  | 113  | 33  | 10 | 1  | 1 | 511  | 421  | 4   | 10 | 4 | 1 | 1361 | 1365 | 7   | 15 | 7 | 1 | 410  | 404  | 17  |
| 4  | 2 | 0 | 615  | 606  | 8   | 10 | 8  | 0 | 391  | 345  | 52  | 11 | 1  | 1 | 168  | 139  | 18  | 11 | 4 | 1 | 647  | 635  | 5   | 16 | 7 | 1 | 905  | 902  | 13  |
| 6  | 2 | 0 | 1538 | 1535 | 10  | 12 | 8  | 0 | 142  | 96   | 71  | 12 | 1  | 1 | 1613 | 1662 | 6   | 12 | 4 | 1 | 1362 | 1347 | 7   | 17 | 7 | 1 | 112  | 82   | 46  |
| 8  | 2 | 0 | 2190 | 2301 | 20  | 14 | 8  | 0 | 902  | 874  | 15  | 13 | 1  | 1 | 238  | 222  | 10  | 13 | 4 | 1 | 725  | 717  | 5   | 18 | 7 | 1 | 41   | 43   | 41  |
| 10 | 2 | 0 | 2653 | 2689 | 15  | 16 | 8  | 0 | 927  | 907  | 15  | 14 | 1  | 1 | 1755 | 1771 | 8   | 14 | 4 | 1 | 1153 | 1140 | 6   | 19 | 7 | 1 | 0    | 36   | 1   |
| 12 | 2 | 0 | 2504 | 2535 | 25  | 18 | 8  | 0 | 2102 | 2102 | 21  | 15 | 1  | 1 | 222  | 176  | 18  | 15 | 4 | 1 | 1694 | 1679 | 11  | 20 | 7 | 1 | 0    | 23   | 1   |
| 14 | 2 | 0 | 1076 | 1049 | 11  | 20 | 8  | 0 | 1463 | 1478 | 32  | 16 | 1  | 1 | 1403 | 1401 | 7   | 16 | 4 | 1 | 879  | 872  | 6   | 21 | 7 | 1 | 246  | 216  | 54  |
| 16 | 2 | 0 | 181  | 172  | 29  | 22 | 8  | 0 | 723  | 726  | 86  | 17 | 1  | 1 | 172  | 46   | 20  | 17 | 4 | 1 | 2024 | 2001 | 9   | 22 | 7 | 1 | 827  | 833  | 12  |
| 18 | 2 | 0 | 284  | 288  | 20  | 24 | 8  | 0 | 275  | 206  | 35  | 18 | 1  | 1 | 403  | 393  | 14  | 18 | 4 | 1 | 736  | 750  | 10  | 23 | 7 | 1 | 131  | 174  | 67  |
| 20 | 2 | 0 | 361  | 321  | 13  | 1  | 9  | 0 | 144  | 85   | 32  | 19 | 1  | 1 | 113  | 137  | 32  | 19 | 4 | 1 | 1466 | 1463 | 9   | 24 | 7 | 1 | 812  | 825  | 13  |
| 22 | 2 | 0 | 305  | 272  | 22  | 3  | 9  | 0 | 1241 | 1242 | 20  | 20 | 1  | 1 | 591  | 606  | 6   | 20 | 4 | 1 | 395  | 405  | 15  | 25 | 7 | 1 | 325  | 240  | 30  |
| 24 | 2 | 0 | 461  | 471  | 20  | 5  | 9  | 0 | 1218 | 1179 | 12  | 21 | 1  | 1 | 149  | 158  | 26  | 21 | 4 | 1 | 1300 | 1316 | 7   | 26 | 7 | 1 | 541  | 489  | 37  |
| 26 | 2 | 0 | 921  | 901  | 11  | 7  | 9  | 0 | 1328 | 1312 | 12  | 22 | 1  | 1 | 859  | 829  | 10  | 22 | 4 | 1 | 338  | 291  | 11  | 0  | 8 | 1 | 381  | 384  | 19  |
| 28 | 2 | 0 | 797  | 825  | 26  | 9  | 9  | 0 | 680  | 662  | 11  | 23 | 1  | 1 | 452  | 405  | 13  | 23 | 4 | 1 | 477  | 488  | 21  | 1  | 8 | 1 | 1522 | 1504 | 9   |
| 1  | 3 | 0 | 3024 | 2999 | 22  | 11 | 9  | 0 | 276  | 305  | 35  | 24 | 1  | 1 | 902  | 892  | 7   | 24 | 4 | 1 | 601  | 582  | 14  | 2  | 8 | 1 | 272  | 271  | 18  |
| 3  | 3 | 0 | 2429 | 2446 | 18  | 13 | 9  | 0 | 814  | 818  | 15  | 25 | 1  | 1 | 203  | 179  | 20  | 25 | 4 | 1 | 339  | 311  | 17  | 3  | 8 | 1 | 516  | 512  | 10  |
| 5  | 3 | 0 | 2370 | 2440 | 22  | 15 | 9  | 0 | 750  | 759  | 32  | 26 | 1  | 1 | 359  | 330  | 21  | 26 | 4 | 1 | 629  | 646  | 10  | 4  | 8 | 1 | 191  | 165  | 20  |
| 7  | 3 | 0 | 1310 | 1336 | 12  | 17 | 9  | 0 | 645  | 665  | 21  | 27 | 1  | 1 | 146  | 109  | 29  | 27 | 4 | 1 | 630  | 594  | 15  | 5  | 8 | 1 | 361  | 338  | 10  |
| 9  | 3 | 0 | 126  | 82   | 19  | 19 | 9  | 0 | 685  | 719  | 41  | 28 | 1  | 1 | 414  | 370  | 23  | 28 | 4 | 1 | 481  | 512  | 44  | 6  | 8 | 1 | 470  | 450  | 11  |
| 11 | 3 | 0 | 1328 | 1346 | 12  | 21 | 9  | 0 | 1174 | 1161 | 17  | 29 | 1  | 1 | 243  | 42   | 64  | 1  | 5 | 1 | 240  | 195  | 19  | 7  | 8 | 1 | 342  | 339  | 26  |
| 13 | 3 | 0 | 1853 | 1888 | 11  | 23 | 9  | 0 | 1027 | 994  | 18  | 0  | 2  | 1 | 1329 | 1315 | 26  | 2  | 5 | 1 | 915  | 936  | 6   | 8  | 8 | 1 | 453  | 424  | 16  |
| 15 | 3 | 0 | 1632 | 1594 | 10  | 0  | 10 | 0 | 511  | 514  | 57  | 1  | 2  | 1 | 412  | 420  | 5   | 3  | 5 | 1 | 614  | 560  | 6   | 9  | 8 | 1 | 666  | 648  | 15  |
| 17 | 3 | 0 | 164  | 181  | 21  | 2  | 10 | 0 | 264  | 200  | 24  | 2  | 2  | 1 | 2302 | 2293 | 12  | 4  | 5 | 1 | 1885 | 1902 | 10  | 10 | 8 | 1 | 490  | 480  | 17  |
| 19 | 3 | 0 | 207  | 164  | 20  | 4  | 10 | 0 | 722  | 684  | 20  | 3  | 2  | 1 | 900  | 899  | 4   | 5  | 5 | 1 | 423  | 385  | 7   | 11 | 8 | 1 | 547  | 555  | 10  |
| 21 | 3 | 0 | 384  | 408  | 12  | 6  | 10 | 0 | 358  | 328  | 19  | 4  | 2  | 1 | 1063 | 1058 | 9   | 6  | 5 | 1 | 927  | 958  | 7   | 12 | 8 | 1 | 403  | 363  | 25  |
| 23 | 3 | 0 | 1108 | 1097 | 11  | 8  | 10 | 0 | 637  | 645  | 33  | 5  | 2  | 1 | 1164 | 1178 | 6   | 7  | 5 | 1 | 573  | 559  | 6   | 13 | 8 | 1 | 114  | 88   | 43  |
| 25 | 3 | 0 | 698  | 686  | 28  | 10 | 10 | 0 | 469  | 445  | 14  | 6  | 2  | 1 | 1217 | 1207 | 8   | 8  | 5 | 1 | 1103 | 1090 | 11  | 14 | 8 | 1 | 168  | 42   |     |

Table 6. 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 |
|----|----|-----|------|------|-----|----|----|---|------|------|-----|----|---|---|------|------|-----|----|---|---|------|------|-----|----|----|---|------|------|-----|
| 22 | 9  | 1   | 488  | 467  | 26  | 3  | 14 | 1 | 198  | 148  | 26  | 1  | 2 | 2 | 1849 | 1855 | 13  | 5  | 5 | 2 | 1213 | 1204 | 9   | 13 | 8  | 2 | 804  | 806  | 12  |
| 23 | 9  | 1   | 183  | 247  | 43  | 4  | 14 | 1 | 169  | 22   | 45  | 2  | 2 | 2 | 1931 | 1968 | 12  | 6  | 5 | 2 | 430  | 455  | 10  | 14 | 8  | 2 | 0    | 131  | 1   |
| 24 | 9  | 1   | 290  | 285  | 30  | 5  | 14 | 1 | 221  | 225  | 45  | 3  | 2 | 2 | 2268 | 2268 | 11  | 7  | 5 | 2 | 602  | 617  | 7   | 15 | 8  | 2 | 586  | 582  | 16  |
| 0  | 10 | 1   | 1007 | 996  | 10  | 6  | 14 | 1 | 247  | 243  | 31  | 4  | 2 | 2 | 314  | 260  | 7   | 8  | 5 | 2 | 885  | 846  | 6   | 16 | 8  | 2 | 563  | 603  | 19  |
| 1  | 10 | 1   | 1115 | 1102 | 7   | 7  | 14 | 1 | 0    | 64   | 1   | 5  | 2 | 2 | 992  | 985  | 6   | 9  | 5 | 2 | 283  | 280  | 17  | 17 | 8  | 2 | 441  | 477  | 12  |
| 2  | 10 | 1   | 650  | 636  | 8   | 8  | 14 | 1 | 155  | 147  | 42  | 6  | 2 | 2 | 738  | 729  | 5   | 10 | 5 | 2 | 554  | 533  | 6   | 18 | 8  | 2 | 980  | 975  | 10  |
| 3  | 10 | 1   | 226  | 229  | 20  | 9  | 14 | 1 | 278  | 99   | 168 | 7  | 2 | 2 | 888  | 887  | 5   | 11 | 5 | 2 | 1076 | 1053 | 7   | 19 | 8  | 2 | 226  | 204  | 55  |
| 4  | 10 | 1   | 1073 | 1071 | 12  | 10 | 14 | 1 | 169  | 189  | 53  | 8  | 2 | 2 | 1315 | 1343 | 7   | 12 | 5 | 2 | 288  | 263  | 17  | 20 | 8  | 2 | 679  | 706  | 15  |
| 5  | 10 | 1   | 565  | 592  | 9   | 11 | 14 | 1 | 261  | 179  | 30  | 9  | 2 | 2 | 921  | 901  | 5   | 13 | 5 | 2 | 1491 | 1455 | 11  | 21 | 8  | 2 | 396  | 432  | 27  |
| 6  | 10 | 1   | 820  | 827  | 9   | 12 | 14 | 1 | 88   | 17   | 88  | 10 | 2 | 2 | 1169 | 1169 | 6   | 14 | 5 | 2 | 169  | 145  | 20  | 22 | 8  | 2 | 115  | 65   | 115 |
| 7  | 10 | 1   | 1644 | 1625 | 10  | 13 | 14 | 1 | 93   | 145  | 93  | 11 | 2 | 2 | 617  | 608  | 6   | 15 | 5 | 2 | 1055 | 1041 | 14  | 23 | 8  | 2 | 414  | 472  | 21  |
| 8  | 10 | 1   | 503  | 523  | 10  | 14 | 14 | 1 | 0    | 94   | 1   | 12 | 2 | 2 | 659  | 639  | 6   | 16 | 5 | 2 | 215  | 193  | 21  | 24 | 8  | 2 | 310  | 239  | 48  |
| 9  | 10 | 1   | 1837 | 1825 | 12  | 1  | 15 | 1 | 198  | 156  | 96  | 13 | 2 | 2 | 774  | 762  | 6   | 17 | 5 | 2 | 181  | 167  | 24  | 25 | 8  | 2 | 447  | 545  | 38  |
| 10 | 10 | 1   | 209  | 202  | 38  | 2  | 15 | 1 | 201  | 122  | 32  | 14 | 2 | 2 | 258  | 280  | 10  | 18 | 5 | 2 | 119  | 102  | 57  | 1  | 9  | 2 | 285  | 302  | 22  |
| 11 | 10 | 1   | 1381 | 1390 | 10  | 3  | 15 | 1 | 277  | 81   | 70  | 15 | 2 | 2 | 1024 | 1018 | 8   | 19 | 5 | 2 | 514  | 477  | 9   | 2  | 9  | 2 | 494  | 497  | 11  |
| 12 | 10 | 1   | 410  | 403  | 14  | 4  | 15 | 1 | 807  | 830  | 18  | 16 | 2 | 2 | 740  | 749  | 6   | 20 | 5 | 2 | 548  | 541  | 12  | 3  | 9  | 2 | 912  | 908  | 7   |
| 13 | 10 | 1   | 745  | 724  | 20  | 5  | 15 | 1 | 44   | 147  | 44  | 17 | 2 | 2 | 756  | 764  | 8   | 21 | 5 | 2 | 830  | 840  | 8   | 4  | 9  | 2 | 323  | 309  | 12  |
| 14 | 10 | 1   | 343  | 330  | 17  | 6  | 15 | 1 | 677  | 697  | 33  | 18 | 2 | 2 | 812  | 823  | 7   | 22 | 5 | 2 | 585  | 559  | 17  | 5  | 9  | 2 | 1013 | 976  | 8   |
| 15 | 10 | 1   | 181  | 163  | 119 | 7  | 15 | 1 | 274  | 154  | 45  | 19 | 2 | 2 | 834  | 831  | 7   | 23 | 5 | 2 | 725  | 707  | 19  | 6  | 9  | 2 | 174  | 177  | 49  |
| 16 | 10 | 1   | 774  | 779  | 12  | 8  | 15 | 1 | 292  | 290  | 45  | 20 | 2 | 2 | 800  | 801  | 7   | 24 | 5 | 2 | 410  | 385  | 17  | 7  | 9  | 2 | 548  | 532  | 10  |
| 17 | 10 | 1   | 538  | 569  | 19  | 9  | 15 | 1 | 87   | 30   | 86  | 21 | 2 | 2 | 535  | 509  | 12  | 25 | 5 | 2 | 671  | 713  | 16  | 8  | 9  | 2 | 331  | 273  | 19  |
| 18 | 10 | 1   | 497  | 531  | 19  | 10 | 15 | 1 | 181  | 161  | 93  | 22 | 2 | 2 | 306  | 307  | 17  | 26 | 5 | 2 | 279  | 288  | 20  | 9  | 9  | 2 | 329  | 295  | 21  |
| 19 | 10 | 1   | 155  | 213  | 80  | 11 | 15 | 1 | 205  | 157  | 56  | 23 | 2 | 2 | 367  | 367  | 12  | 27 | 5 | 2 | 60   | 46   | 59  | 10 | 9  | 2 | 154  | 178  | 38  |
| 20 | 10 | 1   | 542  | 548  | 23  | 0  | 16 | 1 | 130  | 44   | 130 | 24 | 2 | 2 | 131  | 61   | 31  | 0  | 6 | 2 | 2257 | 2281 | 15  | 11 | 9  | 2 | 817  | 811  | 9   |
| 21 | 10 | 1   | 345  | 376  | 20  | 1  | 16 | 1 | 706  | 724  | 22  | 25 | 2 | 2 | 223  | 232  | 18  | 1  | 6 | 2 | 2188 | 2219 | 11  | 12 | 9  | 2 | 438  | 475  | 19  |
| 22 | 10 | 1   | 320  | 410  | 96  | 2  | 16 | 1 | 136  | 84   | 68  | 26 | 2 | 2 | 470  | 468  | 16  | 2  | 6 | 2 | 1230 | 1249 | 7   | 13 | 9  | 2 | 1226 | 1237 | 10  |
| 23 | 10 | 1   | 367  | 388  | 39  | 3  | 16 | 1 | 641  | 660  | 21  | 27 | 2 | 2 | 223  | 53   | 29  | 3  | 6 | 2 | 2054 | 2043 | 11  | 14 | 9  | 2 | 508  | 480  | 28  |
| 1  | 11 | 1   | 358  | 355  | 19  | 4  | 16 | 1 | 271  | 275  | 63  | 28 | 2 | 2 | 338  | 343  | 21  | 4  | 6 | 2 | 148  | 80   | 30  | 15 | 9  | 2 | 1023 | 1042 | 10  |
| 2  | 11 | 1   | 764  | 779  | 10  | 5  | 16 | 1 | 229  | 174  | 43  | 1  | 3 | 2 | 1306 | 1310 | 7   | 5  | 6 | 2 | 1684 | 1631 | 9   | 16 | 9  | 2 | 483  | 486  | 16  |
| 3  | 11 | 1   | 479  | 482  | 9   | 0  | 0  | 2 | 2686 | 2657 | 29  | 2  | 3 | 2 | 883  | 842  | 7   | 6  | 6 | 2 | 592  | 581  | 6   | 17 | 9  | 2 | 355  | 393  | 26  |
| 4  | 11 | 1   | 416  | 433  | 10  | 1  | 0  | 2 | 703  | 633  | 6   | 3  | 3 | 2 | 1570 | 1629 | 9   | 7  | 6 | 2 | 916  | 925  | 6   | 18 | 9  | 2 | 447  | 377  | 21  |
| 5  | 11 | 1   | 374  | 414  | 16  | 2  | 0  | 2 | 1331 | 1368 | 8   | 4  | 3 | 2 | 834  | 844  | 5   | 8  | 6 | 2 | 975  | 989  | 8   | 19 | 9  | 2 | 226  | 128  | 32  |
| 6  | 11 | 1   | 303  | 166  | 34  | 3  | 0  | 2 | 3219 | 3180 | 18  | 5  | 3 | 2 | 1085 | 1176 | 9   | 9  | 6 | 2 | 763  | 768  | 6   | 20 | 9  | 2 | 115  | 61   | 115 |
| 7  | 11 | 1   | 188  | 22   | 35  | 4  | 0  | 2 | 980  | 952  | 5   | 6  | 3 | 2 | 1283 | 1282 | 7   | 10 | 6 | 2 | 1590 | 1567 | 8   | 21 | 9  | 2 | 528  | 600  | 20  |
| 8  | 11 | 1   | 27   | 50   | 27  | 5  | 0  | 2 | 1899 | 1932 | 19  | 7  | 3 | 2 | 769  | 810  | 6   | 11 | 6 | 2 | 759  | 752  | 9   | 22 | 9  | 2 | 72   | 19   | 72  |
| 9  | 11 | 1   | 144  | 111  | 35  | 6  | 0  | 2 | 880  | 900  | 8   | 8  | 3 | 2 | 759  | 738  | 5   | 12 | 6 | 2 | 1022 | 999  | 9   | 23 | 9  | 2 | 757  | 724  | 19  |
| 10 | 11 | 1   | 266  | 231  | 37  | 7  | 0  | 2 | 2105 | 2155 | 17  | 9  | 3 | 2 | 284  | 216  | 12  | 13 | 6 | 2 | 555  | 545  | 10  | 0  | 10 | 2 | 295  | 262  | 23  |
| 11 | 11 | 1   | 245  | 173  | 19  | 8  | 0  | 2 | 2547 | 2578 | 16  | 10 | 3 | 2 | 168  | 112  | 24  | 14 | 6 | 2 | 75   | 115  | 75  | 1  | 10 | 2 | 429  | 385  | 16  |
| 12 | 11 | 1   | 421  | 404  | 15  | 9  | 0  | 2 | 2838 | 2879 | 14  | 11 | 3 | 2 | 1050 | 1069 | 7   | 15 | 6 | 2 | 966  | 934  | 12  | 2  | 10 | 2 | 541  | 556  | 14  |
| 13 | 11 | 1   | 173  | 276  | 80  | 10 | 0  | 2 | 2175 | 2233 | 10  | 12 | 3 | 2 | 87   | 82   | 86  | 16 | 6 | 2 | 994  | 963  | 8   | 3  | 10 | 2 | 88   | 39   | 45  |
| 14 | 11 | 1   | 625  | 661  | 21  | 11 | 0  | 2 | 1985 | 2032 | 10  | 13 | 3 | 2 | 1826 | 1835 | 9   | 17 | 6 | 2 | 1197 | 1200 | 9   | 4  | 10 | 2 | 419  | 417  | 24  |
| 15 | 11 | 1   | 197  | 153  | 60  | 12 | 0  | 2 | 1674 | 1694 | 9   | 14 | 3 | 2 | 505  | 506  | 11  | 18 | 6 | 2 | 1340 | 1345 | 9   | 5  | 10 | 2 | 260  | 281  | 16  |
| 16 | 11 | 1   | 127  | 27   | 68  | 13 | 0  | 2 | 1521 | 1529 | 8   | 15 | 3 | 2 | 1411 | 1397 | 7   | 19 | 6 | 2 | 751  | 759  | 9   | 6  | 10 | 2 | 123  | 107  | 103 |
| 17 | 11 | 1   | 305  | 272  | 49  | 14 | 0  | 2 | 77   | 39   | 77  | 16 | 3 | 2 | 398  | 401  | 7   | 20 | 6 | 2 | 1227 | 1236 | 9   | 7  | 10 | 2 | 363  | 313  | 34  |
| 18 | 11 | 1   | 125  | 72   | 77  | 15 | 0  | 2 | 1197 | 1183 | 8   | 17 | 3 | 2 | 435  | 444  | 12  | 21 | 6 | 2 | 688  | 672  | 13  | 8  | 10 | 2 | 440  | 476  | 12  |
| 19 | 11 | 1   | 341  | 90   | 46  | 16 | 0  | 2 | 1202 | 1192 | 9   | 18 | 3 | 2 | 189  | 224  | 15  | 22 | 6 | 2 | 627  | 640  | 15  | 9  | 10 | 2 | 131  | 104  | 67  |
| 20 | 11 | 1   | 218  | 237  | 63  | 17 | 0  | 2 | 576  | 538  | 9   | 19 | 3 | 2 | 431  | 440  | 8   | 23 | 6 | 2 | 566  | 548  | 17  | 10 | 10 | 2 | 181  | 51   | 54  |
| 21 | 11 | 1   | 0    | 246  | 1   | 18 | 0  | 2 | 1196 | 1175 | 13  | 20 | 3 | 2 | 106  | 72   | 35  | 24 | 6 | 2 | 302  | 243  | 31  | 11 | 10 | 2 | 452  | 439  | 15  |
| 0  | 12 | 1   | 387  | 373  | 35  | 19 | 0  | 2 | 588  | 582  | 10  | 21 | 3 | 2 | 918  | 930  | 7   | 25 | 6 | 2 | 93   | 75   | 92  | 12 | 10 | 2 | 185  | 135  | 56  |
| 1  | 12 | 1   | 796  | 771  | 14  | 20 | 0  | 2 | 793  | 789  | 12  | 22 | 3 | 2 | 414  | 381  | 21  | 26 | 6 | 2 | 814  | 797  | 13  | 13 | 10 | 2 | 389  | 399  | 19  |
| 2  | 12 | 1   | 298  | 322  | 19  | 21 | 0  | 2 | 391  | 316  | 32  | 23 | 3 | 2 | 1438 | 1412 | 8   | 1  | 7 | 2 | 148  | 129  | 17  | 14 | 10 | 2 | 172  | 56   | 67  |
| 3  | 12 | 1   | 1030 | 1048 | 9   | 22 | 0  | 2 | 680  | 724  | 13  | 24 | 3 | 2 | 461  | 459  | 10  | 2  | 7 | 2 | 301  | 283  | 24  | 15 | 10 | 2 | 282  | 296  | 28  |
| 4  | 12 | 1   | 650  | 672  | 8   | 23 | 0  | 2 | 751  | 713  | 13  | 25 | 3 | 2 | 778  | 796  | 11  | 3  | 7 | 2 | 222  | 202  | 22  | 16 | 10 | 2 | 24   | 50   | 23  |
| 5  | 12 | 1   | 418  | 438  | 15  | 24 | 0  | 2 | 429  | 354  | 34  | 26 | 3 | 2 | 248  | 249  | 19  | 4  | 7 | 2 | 366  | 363  | 10  | 17 | 10 | 2 | 216  | 277  | 44  |
| 6  | 12 | 1   | 839  | 879  | 10  | 25 | 0  | 2 | 801  | 773  | 25  | 27 | 3 | 2 | 341  | 339  | 21  | 5  | 7 | 2 | 123  | 8    | 24  | 18 | 10 | 2 | 0    | 63   | 1   |
| 7  | 12 | 1   | 140  | 49   | 117 | 26 | 0  | 2 | 650  | 642  | 15  | 0  | 4 | 2 | 738  | 705  | 8   | 6  | 7 | 2 | 236  | 263  | 13  | 19 | 10 | 2 | 309  | 329  | 64  |
| 8  | 12 | 1</ |      |      |     |    |    |   |      |      |     |    |   |   |      |      |     |    |   |   |      |      |     |    |    |   |      |      |     |

Table 6. Observed and calculated structure factors for 1 Page 3

| 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 |
|----|----|---|------|------|-----|----|---|---|------|------|-----|----|---|---|------|------|-----|----|----|---|------|------|-----|----|----|---|------|------|-----|
| 9  | 12 | 2 | 825  | 843  | 12  | 2  | 2 | 3 | 948  | 964  | 7   | 6  | 5 | 3 | 317  | 304  | 13  | 15 | 8  | 3 | 41   | 68   | 40  | 16 | 12 | 3 | 252  | 144  | 110 |
| 10 | 12 | 2 | 917  | 915  | 24  | 3  | 2 | 3 | 1038 | 1098 | 9   | 7  | 5 | 3 | 122  | 22   | 28  | 16 | 8  | 3 | 172  | 151  | 44  | 17 | 12 | 3 | 257  | 80   | 70  |
| 11 | 12 | 2 | 640  | 649  | 18  | 4  | 2 | 3 | 108  | 49   | 20  | 8  | 5 | 3 | 259  | 263  | 13  | 17 | 8  | 3 | 360  | 341  | 20  | 1  | 13 | 3 | 262  | 236  | 63  |
| 12 | 12 | 2 | 449  | 447  | 15  | 5  | 2 | 3 | 319  | 359  | 8   | 9  | 5 | 3 | 183  | 170  | 21  | 18 | 8  | 3 | 221  | 234  | 21  | 2  | 13 | 3 | 523  | 507  | 19  |
| 13 | 12 | 2 | 299  | 336  | 32  | 6  | 2 | 3 | 202  | 195  | 12  | 10 | 5 | 3 | 563  | 556  | 10  | 19 | 8  | 3 | 388  | 379  | 32  | 3  | 13 | 3 | 513  | 500  | 14  |
| 14 | 12 | 2 | 214  | 137  | 52  | 7  | 2 | 3 | 900  | 835  | 5   | 11 | 5 | 3 | 227  | 216  | 14  | 20 | 8  | 3 | 207  | 171  | 32  | 4  | 13 | 3 | 823  | 805  | 29  |
| 15 | 12 | 2 | 257  | 212  | 66  | 8  | 2 | 3 | 121  | 68   | 19  | 12 | 5 | 3 | 1311 | 1319 | 10  | 21 | 8  | 3 | 216  | 13   | 34  | 5  | 13 | 3 | 487  | 487  | 17  |
| 16 | 12 | 2 | 553  | 609  | 36  | 9  | 2 | 3 | 275  | 308  | 9   | 13 | 5 | 3 | 606  | 613  | 7   | 22 | 8  | 3 | 111  | 46   | 96  | 6  | 13 | 3 | 685  | 723  | 11  |
| 17 | 12 | 2 | 161  | 143  | 57  | 10 | 2 | 3 | 659  | 619  | 5   | 14 | 5 | 3 | 1538 | 1557 | 16  | 23 | 8  | 3 | 150  | 34   | 97  | 7  | 13 | 3 | 262  | 223  | 36  |
| 18 | 12 | 2 | 626  | 612  | 20  | 11 | 2 | 3 | 757  | 714  | 5   | 15 | 5 | 3 | 500  | 499  | 8   | 24 | 8  | 3 | 240  | 165  | 65  | 8  | 13 | 3 | 321  | 255  | 20  |
| 19 | 12 | 2 | 286  | 36   | 50  | 12 | 2 | 3 | 120  | 30   | 20  | 16 | 5 | 3 | 773  | 763  | 7   | 1  | 9  | 3 | 295  | 255  | 16  | 9  | 13 | 3 | 194  | 228  | 38  |
| 1  | 13 | 2 | 177  | 11   | 120 | 13 | 2 | 3 | 724  | 753  | 4   | 17 | 5 | 3 | 342  | 328  | 18  | 2  | 9  | 3 | 498  | 503  | 7   | 10 | 13 | 3 | 302  | 285  | 77  |
| 2  | 13 | 2 | 164  | 167  | 39  | 14 | 2 | 3 | 742  | 738  | 8   | 18 | 5 | 3 | 338  | 330  | 17  | 3  | 9  | 3 | 122  | 34   | 48  | 11 | 13 | 3 | 317  | 347  | 20  |
| 3  | 13 | 2 | 314  | 331  | 28  | 15 | 2 | 3 | 1958 | 1987 | 9   | 19 | 5 | 3 | 232  | 160  | 29  | 4  | 9  | 3 | 928  | 930  | 10  | 12 | 13 | 3 | 770  | 762  | 13  |
| 4  | 13 | 2 | 64   | 96   | 63  | 16 | 2 | 3 | 874  | 869  | 13  | 20 | 5 | 3 | 169  | 42   | 34  | 5  | 9  | 3 | 262  | 213  | 23  | 13 | 13 | 3 | 474  | 432  | 37  |
| 5  | 13 | 2 | 218  | 269  | 45  | 17 | 2 | 3 | 1691 | 1686 | 9   | 21 | 5 | 3 | 263  | 258  | 26  | 6  | 9  | 3 | 1068 | 1047 | 11  | 14 | 13 | 3 | 880  | 908  | 15  |
| 6  | 13 | 2 | 330  | 320  | 20  | 18 | 2 | 3 | 883  | 842  | 7   | 22 | 5 | 3 | 273  | 262  | 20  | 7  | 9  | 3 | 226  | 214  | 40  | 15 | 13 | 3 | 487  | 508  | 46  |
| 7  | 13 | 2 | 311  | 316  | 21  | 19 | 2 | 3 | 1326 | 1307 | 8   | 23 | 5 | 3 | 353  | 365  | 32  | 8  | 9  | 3 | 551  | 556  | 12  | 0  | 14 | 3 | 187  | 178  | 186 |
| 8  | 13 | 2 | 241  | 235  | 47  | 20 | 2 | 3 | 993  | 1015 | 9   | 24 | 5 | 3 | 450  | 458  | 21  | 9  | 9  | 3 | 175  | 65   | 59  | 1  | 14 | 3 | 218  | 112  | 29  |
| 9  | 13 | 2 | 383  | 385  | 17  | 21 | 2 | 3 | 1192 | 1212 | 9   | 25 | 5 | 3 | 395  | 376  | 25  | 10 | 9  | 3 | 241  | 219  | 20  | 2  | 14 | 3 | 199  | 162  | 30  |
| 10 | 13 | 2 | 156  | 30   | 155 | 22 | 2 | 3 | 758  | 761  | 13  | 26 | 5 | 3 | 108  | 54   | 83  | 11 | 9  | 3 | 240  | 85   | 46  | 3  | 14 | 3 | 218  | 76   | 35  |
| 11 | 13 | 2 | 162  | 154  | 162 | 23 | 2 | 3 | 567  | 566  | 18  | 27 | 5 | 3 | 256  | 69   | 66  | 12 | 9  | 3 | 237  | 67   | 37  | 4  | 14 | 3 | 226  | 195  | 84  |
| 12 | 13 | 2 | 178  | 187  | 91  | 24 | 2 | 3 | 363  | 342  | 23  | 0  | 6 | 3 | 404  | 412  | 11  | 13 | 9  | 3 | 332  | 389  | 16  | 5  | 14 | 3 | 150  | 137  | 149 |
| 13 | 13 | 2 | 37   | 145  | 36  | 25 | 2 | 3 | 371  | 329  | 25  | 1  | 6 | 3 | 1115 | 1111 | 6   | 14 | 9  | 3 | 442  | 365  | 17  | 6  | 14 | 3 | 269  | 106  | 54  |
| 14 | 13 | 2 | 188  | 78   | 187 | 26 | 2 | 3 | 270  | 211  | 34  | 2  | 6 | 3 | 908  | 908  | 6   | 15 | 9  | 3 | 279  | 359  | 24  | 7  | 14 | 3 | 291  | 237  | 23  |
| 15 | 13 | 2 | 211  | 115  | 46  | 27 | 2 | 3 | 519  | 524  | 11  | 3  | 6 | 3 | 1121 | 1115 | 7   | 16 | 9  | 3 | 282  | 297  | 20  | 8  | 14 | 3 | 144  | 124  | 67  |
| 16 | 13 | 2 | 154  | 168  | 71  | 28 | 2 | 3 | 189  | 136  | 92  | 4  | 6 | 3 | 586  | 586  | 6   | 17 | 9  | 3 | 153  | 187  | 61  | 9  | 14 | 3 | 305  | 290  | 29  |
| 17 | 13 | 2 | 182  | 47   | 89  | 1  | 3 | 3 | 185  | 156  | 9   | 5  | 6 | 3 | 514  | 511  | 8   | 18 | 9  | 3 | 72   | 22   | 71  | 10 | 14 | 3 | 157  | 117  | 59  |
| 0  | 14 | 2 | 1127 | 1095 | 17  | 2  | 3 | 3 | 94   | 60   | 11  | 6  | 6 | 3 | 292  | 297  | 14  | 19 | 9  | 3 | 157  | 106  | 80  | 11 | 14 | 3 | 269  | 234  | 28  |
| 1  | 14 | 2 | 1072 | 1036 | 12  | 3  | 3 | 3 | 264  | 240  | 6   | 7  | 6 | 3 | 263  | 239  | 11  | 20 | 9  | 3 | 512  | 528  | 15  | 12 | 14 | 3 | 223  | 139  | 68  |
| 2  | 14 | 2 | 844  | 817  | 13  | 4  | 3 | 3 | 585  | 540  | 5   | 8  | 6 | 3 | 56   | 55   | 56  | 21 | 9  | 3 | 185  | 300  | 53  | 13 | 14 | 3 | 223  | 185  | 77  |
| 3  | 14 | 2 | 742  | 786  | 12  | 5  | 3 | 3 | 184  | 179  | 9   | 9  | 6 | 3 | 111  | 126  | 53  | 22 | 9  | 3 | 550  | 486  | 108 | 1  | 15 | 3 | 256  | 138  | 42  |
| 4  | 14 | 2 | 404  | 418  | 22  | 6  | 3 | 3 | 629  | 600  | 5   | 10 | 6 | 3 | 343  | 329  | 18  | 0  | 10 | 3 | 1397 | 1390 | 13  | 2  | 15 | 3 | 575  | 531  | 32  |
| 5  | 14 | 2 | 570  | 603  | 19  | 7  | 3 | 3 | 487  | 465  | 5   | 11 | 6 | 3 | 809  | 786  | 8   | 1  | 10 | 3 | 1787 | 1781 | 18  | 3  | 15 | 3 | 421  | 354  | 54  |
| 6  | 14 | 2 | 509  | 499  | 15  | 8  | 3 | 3 | 105  | 57   | 29  | 12 | 6 | 3 | 129  | 21   | 24  | 2  | 10 | 3 | 921  | 923  | 11  | 4  | 15 | 3 | 629  | 651  | 15  |
| 7  | 14 | 2 | 450  | 400  | 26  | 9  | 3 | 3 | 177  | 155  | 8   | 13 | 6 | 3 | 347  | 355  | 17  | 3  | 10 | 3 | 1383 | 1374 | 10  | 5  | 15 | 3 | 357  | 328  | 52  |
| 8  | 14 | 2 | 899  | 886  | 11  | 10 | 3 | 3 | 764  | 729  | 5   | 14 | 6 | 3 | 164  | 49   | 33  | 4  | 10 | 3 | 361  | 390  | 16  | 6  | 15 | 3 | 593  | 571  | 23  |
| 9  | 14 | 2 | 392  | 345  | 46  | 11 | 3 | 3 | 144  | 25   | 23  | 15 | 6 | 3 | 539  | 512  | 9   | 5  | 10 | 3 | 596  | 587  | 18  | 7  | 15 | 3 | 106  | 99   | 106 |
| 10 | 14 | 2 | 647  | 675  | 17  | 12 | 3 | 3 | 431  | 436  | 10  | 16 | 6 | 3 | 206  | 172  | 29  | 6  | 10 | 3 | 117  | 106  | 67  | 8  | 15 | 3 | 452  | 300  | 132 |
| 11 | 14 | 2 | 292  | 315  | 38  | 13 | 3 | 3 | 166  | 108  | 19  | 17 | 6 | 3 | 697  | 690  | 8   | 7  | 10 | 3 | 241  | 234  | 49  | 9  | 15 | 3 | 280  | 207  | 57  |
| 12 | 14 | 2 | 366  | 284  | 54  | 14 | 3 | 3 | 616  | 608  | 7   | 18 | 6 | 3 | 548  | 543  | 9   | 8  | 10 | 3 | 424  | 440  | 13  | 0  | 0  | 4 | 537  | 530  | 14  |
| 13 | 14 | 2 | 507  | 490  | 37  | 15 | 3 | 3 | 120  | 101  | 31  | 19 | 6 | 3 | 827  | 835  | 11  | 9  | 10 | 3 | 283  | 280  | 29  | 1  | 0  | 4 | 562  | 638  | 8   |
| 14 | 14 | 2 | 184  | 58   | 89  | 16 | 3 | 3 | 414  | 392  | 14  | 20 | 6 | 3 | 533  | 541  | 10  | 10 | 10 | 3 | 198  | 70   | 32  | 2  | 0  | 4 | 473  | 440  | 8   |
| 1  | 15 | 2 | 252  | 244  | 36  | 17 | 3 | 3 | 251  | 255  | 14  | 21 | 6 | 3 | 309  | 263  | 46  | 11 | 10 | 3 | 105  | 143  | 58  | 3  | 0  | 4 | 870  | 897  | 6   |
| 2  | 15 | 2 | 108  | 66   | 108 | 18 | 3 | 3 | 542  | 549  | 11  | 22 | 6 | 3 | 240  | 234  | 25  | 12 | 10 | 3 | 239  | 224  | 22  | 4  | 0  | 4 | 1314 | 1297 | 12  |
| 3  | 15 | 2 | 655  | 677  | 17  | 19 | 3 | 3 | 164  | 173  | 38  | 23 | 6 | 3 | 144  | 73   | 50  | 13 | 10 | 3 | 453  | 447  | 23  | 5  | 0  | 4 | 150  | 112  | 15  |
| 4  | 15 | 2 | 257  | 304  | 39  | 20 | 3 | 3 | 322  | 321  | 17  | 24 | 6 | 3 | 198  | 97   | 39  | 14 | 10 | 3 | 285  | 332  | 23  | 6  | 0  | 4 | 3442 | 3492 | 19  |
| 5  | 15 | 2 | 518  | 543  | 26  | 21 | 3 | 3 | 82   | 122  | 81  | 25 | 6 | 3 | 51   | 17   | 50  | 15 | 10 | 3 | 949  | 951  | 12  | 7  | 0  | 4 | 1123 | 1109 | 7   |
| 6  | 15 | 2 | 276  | 310  | 56  | 22 | 3 | 3 | 275  | 259  | 24  | 1  | 7 | 3 | 424  | 422  | 12  | 16 | 10 | 3 | 656  | 654  | 14  | 8  | 0  | 4 | 2811 | 2880 | 16  |
| 7  | 15 | 2 | 355  | 378  | 20  | 23 | 3 | 3 | 181  | 66   | 42  | 2  | 7 | 3 | 916  | 913  | 8   | 17 | 10 | 3 | 1395 | 1365 | 17  | 9  | 0  | 4 | 790  | 802  | 6   |
| 8  | 15 | 2 | 204  | 118  | 46  | 24 | 3 | 3 | 334  | 328  | 19  | 3  | 7 | 3 | 689  | 677  | 10  | 18 | 10 | 3 | 866  | 856  | 12  | 10 | 0  | 4 | 2663 | 2722 | 16  |
| 9  | 15 | 2 | 142  | 32   | 141 | 25 | 3 | 3 | 123  | 47   | 45  | 4  | 7 | 3 | 1632 | 1611 | 9   | 19 | 10 | 3 | 1371 | 1369 | 20  | 11 | 0  | 4 | 427  | 430  | 6   |
| 10 | 15 | 2 | 118  | 41   | 118 | 26 | 3 | 3 | 354  | 390  | 24  | 5  | 7 | 3 | 938  | 911  | 7   | 20 | 10 | 3 | 722  | 710  | 17  | 12 | 0  | 4 | 2170 | 2202 | 11  |
| 0  | 16 | 2 | 390  | 338  | 28  | 27 | 3 | 3 | 137  | 26   | 51  | 6  | 7 | 3 | 1638 | 1621 | 11  | 21 | 10 | 3 | 890  | 929  | 23  | 13 | 0  | 4 | 274  | 303  | 11  |
| 1  | 16 | 2 | 334  | 358  | 32  | 28 | 3 | 3 | 252  | 140  | 61  | 7  | 7 | 3 | 711  | 698  | 7   | 1  | 11 | 3 | 194  | 169  | 39  | 14 | 0  | 4 | 1030 | 1021 | 12  |
| 2  | 16 | 2 | 435  | 333  | 52  | 0  | 4 | 3 | 695  | 674  | 8   | 8  | 7 | 3 | 524  | 530  | 12  | 2  | 11 | 3 | 292  | 271  | 27  | 15 | 0  | 4 | 914  | 909  | 9   |
| 3  | 16 | 2 | 274  | 280  | 97  | 1  |   |   |      |      |     |    |   |   |      |      |     |    |    |   |      |      |     |    |    |   |      |      |     |

Table 6. 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 |      |      |     |    |   |   |      |      |     |
|---------------------|---|---|------|------|---------------------|----|---|---|------|---------------------|-----|----|----|---|---------------------|------|-----|----|----|---------------------|------|------|-----|----|---|---|------|------|-----|
| 21                  | 1 | 4 | 169  | 61   | 72                  | 26 | 4 | 4 | 326  | 335                 | 20  | 11 | 8  | 4 | 386                 | 372  | 22  | 13 | 12 | 4                   | 79   | 184  | 79  | 22 | 2 | 5 | 139  | 62   | 102 |
| 22                  | 1 | 4 | 524  | 526  | 14                  | 1  | 5 | 4 | 719  | 688                 | 5   | 12 | 8  | 4 | 1346                | 1336 | 10  | 14 | 12 | 4                   | 242  | 202  | 80  | 23 | 2 | 5 | 272  | 300  | 21  |
| 23                  | 1 | 4 | 161  | 52   | 98                  | 2  | 5 | 4 | 600  | 588                 | 4   | 13 | 8  | 4 | 90                  | 106  | 89  | 15 | 12 | 4                   | 309  | 338  | 26  | 24 | 2 | 5 | 484  | 450  | 15  |
| 24                  | 1 | 4 | 492  | 480  | 22                  | 3  | 5 | 4 | 1086 | 1066                | 6   | 14 | 8  | 4 | 771                 | 766  | 12  | 16 | 12 | 4                   | 227  | 163  | 62  | 25 | 2 | 5 | 279  | 228  | 44  |
| 25                  | 1 | 4 | 199  | 28   | 88                  | 4  | 5 | 4 | 1063 | 1041                | 5   | 15 | 8  | 4 | 534                 | 541  | 22  | 17 | 12 | 4                   | 387  | 466  | 28  | 26 | 2 | 5 | 655  | 658  | 20  |
| 26                  | 1 | 4 | 243  | 268  | 21                  | 5  | 5 | 4 | 894  | 909                 | 7   | 16 | 8  | 4 | 170                 | 163  | 57  | 1  | 13 | 4                   | 207  | 236  | 29  | 1  | 3 | 5 | 499  | 463  | 10  |
| 27                  | 1 | 4 | 226  | 262  | 41                  | 6  | 5 | 4 | 918  | 907                 | 6   | 17 | 8  | 4 | 719                 | 733  | 11  | 2  | 13 | 4                   | 263  | 4    | 51  | 2  | 3 | 5 | 165  | 105  | 16  |
| 0                   | 2 | 4 | 2448 | 2449 | 34                  | 7  | 5 | 4 | 673  | 686                 | 13  | 18 | 8  | 4 | 148                 | 58   | 148 | 3  | 13 | 4                   | 157  | 142  | 73  | 3  | 3 | 5 | 246  | 274  | 15  |
| 1                   | 2 | 4 | 318  | 310  | 11                  | 8  | 5 | 4 | 414  | 411                 | 7   | 19 | 8  | 4 | 682                 | 647  | 11  | 4  | 13 | 4                   | 359  | 306  | 21  | 4  | 3 | 5 | 465  | 466  | 9   |
| 2                   | 2 | 4 | 1925 | 1973 | 18                  | 9  | 5 | 4 | 175  | 131                 | 15  | 20 | 8  | 4 | 83                  | 74   | 83  | 5  | 13 | 4                   | 355  | 356  | 30  | 5  | 3 | 5 | 294  | 276  | 8   |
| 3                   | 2 | 4 | 159  | 119  | 8                   | 10 | 5 | 4 | 124  | 13                  | 27  | 21 | 8  | 4 | 559                 | 581  | 15  | 6  | 13 | 4                   | 327  | 318  | 35  | 6  | 3 | 5 | 374  | 362  | 9   |
| 4                   | 2 | 4 | 1236 | 1247 | 9                   | 11 | 5 | 4 | 120  | 81                  | 24  | 22 | 8  | 4 | 73                  | 46   | 73  | 7  | 13 | 4                   | 191  | 162  | 191 | 7  | 3 | 5 | 572  | 526  | 7   |
| 5                   | 2 | 4 | 520  | 520  | 7                   | 12 | 5 | 4 | 623  | 596                 | 7   | 23 | 8  | 4 | 63                  | 81   | 62  | 8  | 13 | 4                   | 208  | 150  | 39  | 8  | 3 | 5 | 155  | 138  | 23  |
| 6                   | 2 | 4 | 1323 | 1269 | 7                   | 13 | 5 | 4 | 502  | 503                 | 16  | 1  | 9  | 4 | 405                 | 425  | 14  | 9  | 13 | 4                   | 167  | 65   | 85  | 9  | 3 | 5 | 462  | 465  | 7   |
| 7                   | 2 | 4 | 457  | 462  | 5                   | 14 | 5 | 4 | 941  | 931                 | 11  | 2  | 9  | 4 | 590                 | 605  | 16  | 10 | 13 | 4                   | 140  | 73   | 139 | 10 | 3 | 5 | 151  | 136  | 18  |
| 8                   | 2 | 4 | 138  | 38   | 12                  | 15 | 5 | 4 | 665  | 655                 | 16  | 3  | 9  | 4 | 931                 | 904  | 9   | 11 | 13 | 4                   | 80   | 30   | 79  | 11 | 3 | 5 | 321  | 313  | 10  |
| 9                   | 2 | 4 | 856  | 857  | 6                   | 16 | 5 | 4 | 468  | 424                 | 19  | 4  | 9  | 4 | 716                 | 706  | 9   | 12 | 13 | 4                   | 0    | 121  | 1   | 12 | 3 | 5 | 260  | 228  | 23  |
| 10                  | 2 | 4 | 261  | 244  | 8                   | 17 | 5 | 4 | 114  | 109                 | 39  | 5  | 9  | 4 | 723                 | 736  | 10  | 13 | 13 | 4                   | 183  | 133  | 105 | 13 | 3 | 5 | 75   | 28   | 75  |
| 11                  | 2 | 4 | 675  | 682  | 6                   | 18 | 5 | 4 | 96   | 58                  | 95  | 6  | 9  | 4 | 577                 | 565  | 14  | 14 | 13 | 4                   | 115  | 108  | 114 | 14 | 3 | 5 | 196  | 171  | 17  |
| 12                  | 2 | 4 | 108  | 40   | 28                  | 19 | 5 | 4 | 390  | 375                 | 13  | 7  | 9  | 4 | 402                 | 377  | 14  | 15 | 13 | 4                   | 180  | 83   | 158 | 15 | 3 | 5 | 267  | 262  | 13  |
| 13                  | 2 | 4 | 320  | 328  | 11                  | 20 | 5 | 4 | 153  | 5                   | 35  | 8  | 9  | 4 | 371                 | 326  | 22  | 0  | 14 | 4                   | 1321 | 1317 | 18  | 16 | 3 | 5 | 375  | 383  | 13  |
| 14                  | 2 | 4 | 495  | 495  | 7                   | 21 | 5 | 4 | 612  | 617                 | 15  | 9  | 9  | 4 | 201                 | 161  | 45  | 1  | 14 | 4                   | 173  | 246  | 62  | 17 | 3 | 5 | 350  | 321  | 18  |
| 15                  | 2 | 4 | 310  | 281  | 11                  | 22 | 5 | 4 | 268  | 288                 | 32  | 10 | 9  | 4 | 93                  | 130  | 93  | 2  | 14 | 4                   | 1176 | 1189 | 13  | 18 | 3 | 5 | 111  | 9    | 48  |
| 16                  | 2 | 4 | 1128 | 1123 | 10                  | 23 | 5 | 4 | 979  | 999                 | 15  | 11 | 9  | 4 | 517                 | 515  | 13  | 3  | 14 | 4                   | 391  | 319  | 53  | 19 | 3 | 5 | 680  | 682  | 11  |
| 17                  | 2 | 4 | 285  | 292  | 19                  | 24 | 5 | 4 | 467  | 473                 | 25  | 12 | 9  | 4 | 589                 | 606  | 22  | 4  | 14 | 4                   | 974  | 917  | 18  | 20 | 3 | 5 | 309  | 255  | 34  |
| 18                  | 2 | 4 | 1102 | 1099 | 10                  | 25 | 5 | 4 | 680  | 707                 | 18  | 13 | 9  | 4 | 1164                | 1174 | 11  | 5  | 14 | 4                   | 143  | 83   | 74  | 21 | 3 | 5 | 626  | 686  | 12  |
| 19                  | 2 | 4 | 477  | 471  | 14                  | 26 | 5 | 4 | 115  | 267                 | 115 | 14 | 9  | 4 | 747                 | 758  | 16  | 6  | 14 | 4                   | 192  | 160  | 84  | 22 | 3 | 5 | 240  | 122  | 35  |
| 20                  | 2 | 4 | 946  | 949  | 9                   | 0  | 6 | 4 | 3019 | 3070                | 17  | 15 | 9  | 4 | 900                 | 895  | 12  | 7  | 14 | 4                   | 647  | 699  | 16  | 23 | 3 | 5 | 520  | 527  | 22  |
| 21                  | 2 | 4 | 207  | 209  | 36                  | 1  | 6 | 4 | 954  | 936                 | 6   | 16 | 9  | 4 | 132                 | 208  | 50  | 8  | 14 | 4                   | 304  | 245  | 61  | 24 | 3 | 5 | 191  | 136  | 50  |
| 22                  | 2 | 4 | 642  | 664  | 10                  | 2  | 6 | 4 | 2447 | 2472                | 17  | 17 | 9  | 4 | 224                 | 260  | 49  | 9  | 14 | 4                   | 670  | 692  | 14  | 25 | 3 | 5 | 375  | 344  | 27  |
| 23                  | 2 | 4 | 122  | 70   | 57                  | 3  | 6 | 4 | 253  | 224                 | 23  | 18 | 9  | 4 | 220                 | 187  | 38  | 10 | 14 | 4                   | 292  | 178  | 37  | 26 | 3 | 5 | 318  | 7    | 42  |
| 24                  | 2 | 4 | 254  | 217  | 39                  | 4  | 6 | 4 | 1407 | 1384                | 11  | 19 | 9  | 4 | 262                 | 70   | 55  | 11 | 14 | 4                   | 548  | 516  | 35  | 0  | 4 | 5 | 3047 | 3114 | 50  |
| 25                  | 2 | 4 | 419  | 417  | 23                  | 5  | 6 | 4 | 651  | 630                 | 10  | 20 | 9  | 4 | 161                 | 195  | 69  | 12 | 14 | 4                   | 286  | 145  | 37  | 1  | 4 | 5 | 980  | 970  | 10  |
| 26                  | 2 | 4 | 172  | 177  | 36                  | 6  | 6 | 4 | 674  | 669                 | 8   | 21 | 9  | 4 | 279                 | 269  | 22  | 1  | 15 | 4                   | 221  | 136  | 96  | 2  | 4 | 5 | 2443 | 2464 | 15  |
| 27                  | 2 | 4 | 528  | 478  | 22                  | 7  | 6 | 4 | 738  | 758                 | 10  | 22 | 9  | 4 | 358                 | 451  | 132 | 2  | 15 | 4                   | 355  | 207  | 66  | 3  | 4 | 5 | 185  | 193  | 14  |
| 1                   | 3 | 4 | 578  | 597  | 5                   | 8  | 6 | 4 | 182  | 89                  | 30  | 0  | 10 | 4 | 212                 | 30   | 45  | 3  | 15 | 4                   | 512  | 434  | 49  | 4  | 4 | 5 | 1694 | 1693 | 10  |
| 2                   | 3 | 4 | 1081 | 1090 | 8                   | 9  | 6 | 4 | 1118 | 1114                | 9   | 1  | 10 | 4 | 342                 | 358  | 19  | 4  | 15 | 4                   | 278  | 165  | 56  | 5  | 4 | 5 | 570  | 539  | 6   |
| 3                   | 3 | 4 | 1612 | 1607 | 10                  | 10 | 6 | 4 | 664  | 668                 | 10  | 2  | 10 | 4 | 548                 | 536  | 12  | 5  | 15 | 4                   | 481  | 395  | 41  | 6  | 4 | 5 | 693  | 683  | 7   |
| 4                   | 3 | 4 | 1246 | 1250 | 7                   | 11 | 6 | 4 | 954  | 942                 | 12  | 3  | 10 | 4 | 187                 | 182  | 25  | 6  | 15 | 4                   | 0    | 124  | 1   | 7  | 4 | 5 | 1050 | 1040 | 10  |
| 5                   | 3 | 4 | 1627 | 1629 | 13                  | 12 | 6 | 4 | 177  | 65                  | 37  | 4  | 10 | 4 | 531                 | 548  | 17  | 7  | 15 | 4                   | 396  | 400  | 42  | 8  | 4 | 5 | 245  | 210  | 12  |
| 6                   | 3 | 4 | 928  | 906  | 9                   | 13 | 6 | 4 | 266  | 172                 | 26  | 5  | 10 | 4 | 0                   | 39   | 1   | 1  | 1  | 5                   | 980  | 935  | 4   | 9  | 4 | 5 | 1418 | 1417 | 9   |
| 7                   | 3 | 4 | 661  | 699  | 7                   | 14 | 6 | 4 | 1118 | 1132                | 16  | 6  | 10 | 4 | 67                  | 67   | 66  | 2  | 1  | 5                   | 1413 | 1373 | 10  | 10 | 4 | 5 | 234  | 183  | 14  |
| 8                   | 3 | 4 | 286  | 307  | 12                  | 15 | 6 | 4 | 349  | 347                 | 12  | 7  | 10 | 4 | 345                 | 297  | 25  | 3  | 1  | 5                   | 1040 | 1027 | 8   | 11 | 4 | 5 | 1449 | 1448 | 11  |
| 9                   | 3 | 4 | 204  | 189  | 30                  | 16 | 6 | 4 | 1335 | 1334                | 9   | 8  | 10 | 4 | 75                  | 105  | 74  | 4  | 1  | 5                   | 1363 | 1332 | 6   | 12 | 4 | 5 | 275  | 226  | 13  |
| 10                  | 3 | 4 | 459  | 444  | 11                  | 17 | 6 | 4 | 532  | 525                 | 18  | 9  | 10 | 4 | 173                 | 214  | 86  | 5  | 1  | 5                   | 996  | 1009 | 5   | 13 | 4 | 5 | 424  | 423  | 16  |
| 11                  | 3 | 4 | 909  | 904  | 7                   | 18 | 6 | 4 | 1287 | 1269                | 9   | 10 | 10 | 4 | 296                 | 295  | 18  | 6  | 1  | 5                   | 1264 | 1260 | 6   | 14 | 4 | 5 | 695  | 702  | 17  |
| 12                  | 3 | 4 | 1153 | 1130 | 8                   | 19 | 6 | 4 | 454  | 455                 | 18  | 11 | 10 | 4 | 191                 | 57   | 45  | 7  | 1  | 5                   | 428  | 437  | 9   | 15 | 4 | 5 | 177  | 97   | 18  |
| 13                  | 3 | 4 | 1331 | 1321 | 8                   | 20 | 6 | 4 | 1113 | 1128                | 13  | 12 | 10 | 4 | 139                 | 163  | 52  | 8  | 1  | 5                   | 906  | 887  | 5   | 16 | 4 | 5 | 1203 | 1184 | 10  |
| 14                  | 3 | 4 | 1082 | 1061 | 7                   | 21 | 6 | 4 | 328  | 353                 | 19  | 13 | 10 | 4 | 225                 | 184  | 56  | 9  | 1  | 5                   | 285  | 258  | 8   | 17 | 4 | 5 | 292  | 261  | 15  |
| 15                  | 3 | 4 | 683  | 680  | 6                   | 22 | 6 | 4 | 662  | 632                 | 16  | 15 | 10 | 4 | 0                   | 104  | 1   | 10 | 1  | 5                   | 117  | 87   | 28  | 18 | 4 | 5 | 1617 | 1615 | 13  |
| 16                  | 3 | 4 | 872  | 890  | 8                   | 23 | 6 | 4 | 101  | 57                  | 101 | 16 | 10 | 4 | 169                 | 193  | 39  | 11 | 1  | 5                   | 940  | 949  | 5   | 19 | 4 | 5 | 296  | 225  | 18  |
| 17                  | 3 | 4 | 223  | 213  | 19                  | 24 | 6 | 4 | 197  | 207                 | 46  | 17 | 10 | 4 | 134                 | 21   | 83  | 12 | 1  | 5                   | 953  | 946  | 7   | 20 | 4 | 5 | 1399 | 1402 | 21  |
| 18                  | 3 | 4 | 285  | 224  | 35                  | 25 | 6 | 4 | 510  | 488                 | 67  | 18 | 10 | 4 | 459                 | 426  | 30  | 13 | 1  | 5                   | 1172 | 1177 | 9   | 21 | 4 | 5 | 171  | 21   | 24  |
| 19                  | 3 | 4 | 420  | 464  | 11                  | 1  | 7 | 4 | 236  | 232                 | 13  | 19 | 10 | 4 | 156                 | 57   | 45  | 14 | 1  | 5                   | 995  | 981  | 10  | 22 | 4 | 5 | 920  | 923  | 17  |
| 20                  | 3 | 4 | 351  | 321  | 24                  | 2  | 7 | 4 | 98   | 87                  | 50  | 20 | 10 | 4 | 346                 | 345  | 67  | 15 | 1  | 5                   | 1103 | 1089 | 10  | 23 | 4 | 5 | 483  | 493  | 16  |
| 21                  | 3 | 4 | 875  | 873  | 19                  | 3  | 7 | 4 | 433  | 423                 | 11  | 21 | 10 | 4 | 302                 | 154  | 57  | 16 | 1  | 5                   | 457  | 419  | 14  | 24 | 4 | 5 | 337  | 290  | 28  |
| 22                  | 3 | 4 | 613  | 608  | 13                  | 4  | 7 | 4 | 91   | 5                   | 90  | 1  | 11 | 4 | 433                 | 453  | 19  | 17 | 1  | 5                   | 353  | 352  | 12  | 25 | 4 | 5 | 760  | 753  | 13  |
| 23                  | 3 | 4 | 888  | 870  | 15                  | 5  | 7 | 4 | 301  | 284                 | 39  | 2  | 11 | 4 | 511                 | 569  | 13  | 18 | 1  | 5                   |      |      |     |    |   |   |      |      |     |

Table 6. 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 |  |  |  |  |  |  |  |  |  |
|---------------------|---|---|------|------|----|----|----|---|------|---------------------|-----|----|---|---|------|------|-----|----|---|---------------------|------|------|----|----|---|---|------|------|-----|---------------------|--|--|--|--|--|--|--|--|--|
| 6                   | 6 | 5 | 605  | 590  | 11 | 2  | 10 | 5 | 128  | 44                  | 41  | 12 | 0 | 6 | 415  | 412  | 19  | 24 | 3 | 6                   | 683  | 682  | 13 | 15 | 7 | 6 | 253  | 215  | 21  |                     |  |  |  |  |  |  |  |  |  |
| 7                   | 6 | 5 | 213  | 156  | 20 | 3  | 10 | 5 | 835  | 832                 | 11  | 13 | 0 | 6 | 556  | 547  | 19  | 25 | 3 | 6                   | 454  | 340  | 31 | 16 | 7 | 6 | 184  | 190  | 26  |                     |  |  |  |  |  |  |  |  |  |
| 8                   | 6 | 5 | 1165 | 1157 | 11 | 4  | 10 | 5 | 366  | 416                 | 16  | 14 | 0 | 6 | 395  | 390  | 14  | 0  | 4 | 6                   | 594  | 580  | 11 | 17 | 7 | 6 | 167  | 41   | 99  |                     |  |  |  |  |  |  |  |  |  |
| 9                   | 6 | 5 | 203  | 227  | 52 | 5  | 10 | 5 | 0    | 65                  | 1   | 15 | 0 | 6 | 1131 | 1123 | 15  | 1  | 4 | 6                   | 799  | 782  | 10 | 18 | 7 | 6 | 126  | 61   | 125 |                     |  |  |  |  |  |  |  |  |  |
| 10                  | 6 | 5 | 1018 | 1006 | 8  | 6  | 10 | 5 | 1079 | 1055                | 16  | 16 | 0 | 6 | 847  | 878  | 12  | 2  | 4 | 6                   | 188  | 136  | 32 | 19 | 7 | 6 | 32   | 111  | 32  |                     |  |  |  |  |  |  |  |  |  |
| 11                  | 6 | 5 | 131  | 59   | 33 | 7  | 10 | 5 | 355  | 410                 | 32  | 17 | 0 | 6 | 1699 | 1701 | 18  | 3  | 4 | 6                   | 466  | 436  | 12 | 20 | 7 | 6 | 169  | 210  | 49  |                     |  |  |  |  |  |  |  |  |  |
| 12                  | 6 | 5 | 714  | 712  | 8  | 8  | 10 | 5 | 1390 | 1365                | 12  | 18 | 0 | 6 | 931  | 930  | 15  | 4  | 4 | 6                   | 145  | 34   | 26 | 21 | 7 | 6 | 0    | 178  | 1   |                     |  |  |  |  |  |  |  |  |  |
| 13                  | 6 | 5 | 191  | 188  | 22 | 9  | 10 | 5 | 440  | 435                 | 15  | 19 | 0 | 6 | 1645 | 1687 | 18  | 5  | 4 | 6                   | 111  | 25   | 36 | 22 | 7 | 6 | 169  | 269  | 102 |                     |  |  |  |  |  |  |  |  |  |
| 14                  | 6 | 5 | 353  | 366  | 13 | 10 | 10 | 5 | 1716 | 1703                | 13  | 20 | 0 | 6 | 909  | 891  | 16  | 6  | 4 | 6                   | 147  | 45   | 47 | 0  | 8 | 6 | 1017 | 986  | 15  |                     |  |  |  |  |  |  |  |  |  |
| 15                  | 6 | 5 | 346  | 325  | 11 | 11 | 10 | 5 | 443  | 456                 | 19  | 21 | 0 | 6 | 1109 | 1124 | 17  | 7  | 4 | 6                   | 377  | 353  | 14 | 1  | 8 | 6 | 1797 | 1748 | 13  |                     |  |  |  |  |  |  |  |  |  |
| 16                  | 6 | 5 | 343  | 323  | 21 | 12 | 10 | 5 | 1282 | 1303                | 18  | 22 | 0 | 6 | 484  | 366  | 21  | 8  | 4 | 6                   | 159  | 42   | 38 | 2  | 8 | 6 | 908  | 919  | 17  |                     |  |  |  |  |  |  |  |  |  |
| 17                  | 6 | 5 | 506  | 515  | 10 | 13 | 10 | 5 | 240  | 245                 | 23  | 23 | 0 | 6 | 426  | 437  | 72  | 9  | 4 | 6                   | 121  | 105  | 38 | 3  | 8 | 6 | 1151 | 1115 | 11  |                     |  |  |  |  |  |  |  |  |  |
| 18                  | 6 | 5 | 134  | 191  | 67 | 14 | 10 | 5 | 507  | 508                 | 15  | 24 | 0 | 6 | 187  | 19   | 187 | 10 | 4 | 6                   | 597  | 597  | 9  | 4  | 8 | 6 | 453  | 454  | 13  |                     |  |  |  |  |  |  |  |  |  |
| 19                  | 6 | 5 | 563  | 576  | 20 | 15 | 10 | 5 | 536  | 557                 | 16  | 25 | 0 | 6 | 437  | 278  | 35  | 11 | 4 | 6                   | 511  | 501  | 8  | 5  | 8 | 6 | 859  | 841  | 19  |                     |  |  |  |  |  |  |  |  |  |
| 20                  | 6 | 5 | 149  | 78   | 56 | 16 | 10 | 5 | 217  | 150                 | 33  | 1  | 1 | 6 | 252  | 233  | 9   | 12 | 4 | 6                   | 157  | 58   | 21 | 6  | 8 | 6 | 161  | 164  | 21  |                     |  |  |  |  |  |  |  |  |  |
| 21                  | 6 | 5 | 266  | 264  | 18 | 17 | 10 | 5 | 837  | 852                 | 13  | 2  | 1 | 6 | 654  | 652  | 4   | 13 | 4 | 6                   | 182  | 106  | 27 | 7  | 8 | 6 | 230  | 243  | 19  |                     |  |  |  |  |  |  |  |  |  |
| 22                  | 6 | 5 | 312  | 287  | 51 | 18 | 10 | 5 | 422  | 384                 | 23  | 3  | 1 | 6 | 589  | 576  | 5   | 14 | 4 | 6                   | 85   | 83   | 58 | 8  | 8 | 6 | 497  | 502  | 27  |                     |  |  |  |  |  |  |  |  |  |
| 23                  | 6 | 5 | 193  | 51   | 42 | 19 | 10 | 5 | 760  | 773                 | 20  | 4  | 1 | 6 | 870  | 864  | 7   | 15 | 4 | 6                   | 176  | 185  | 24 | 9  | 8 | 6 | 355  | 348  | 13  |                     |  |  |  |  |  |  |  |  |  |
| 24                  | 6 | 5 | 336  | 241  | 41 | 20 | 10 | 5 | 0    | 196                 | 1   | 5  | 1 | 6 | 583  | 582  | 6   | 16 | 4 | 6                   | 281  | 308  | 25 | 10 | 8 | 6 | 173  | 195  | 30  |                     |  |  |  |  |  |  |  |  |  |
| 1                   | 7 | 5 | 56   | 110  | 55 | 1  | 11 | 5 | 0    | 24                  | 1   | 6  | 1 | 6 | 673  | 668  | 5   | 17 | 4 | 6                   | 367  | 376  | 15 | 11 | 8 | 6 | 333  | 364  | 23  |                     |  |  |  |  |  |  |  |  |  |
| 2                   | 7 | 5 | 750  | 755  | 8  | 2  | 11 | 5 | 179  | 181                 | 36  | 7  | 1 | 6 | 162  | 100  | 19  | 18 | 4 | 6                   | 219  | 137  | 23 | 12 | 8 | 6 | 222  | 118  | 24  |                     |  |  |  |  |  |  |  |  |  |
| 3                   | 7 | 5 | 720  | 711  | 10 | 3  | 11 | 5 | 506  | 464                 | 18  | 8  | 1 | 6 | 1005 | 1013 | 9   | 19 | 4 | 6                   | 350  | 347  | 30 | 13 | 8 | 6 | 423  | 417  | 27  |                     |  |  |  |  |  |  |  |  |  |
| 4                   | 7 | 5 | 1455 | 1441 | 8  | 4  | 11 | 5 | 225  | 239                 | 50  | 9  | 1 | 6 | 125  | 127  | 21  | 20 | 4 | 6                   | 162  | 206  | 74 | 14 | 8 | 6 | 363  | 364  | 23  |                     |  |  |  |  |  |  |  |  |  |
| 5                   | 7 | 5 | 956  | 924  | 9  | 5  | 11 | 5 | 192  | 179                 | 31  | 10 | 1 | 6 | 252  | 245  | 23  | 21 | 4 | 6                   | 51   | 99   | 50 | 15 | 8 | 6 | 955  | 981  | 10  |                     |  |  |  |  |  |  |  |  |  |
| 6                   | 7 | 5 | 1148 | 1141 | 8  | 6  | 11 | 5 | 273  | 152                 | 28  | 11 | 1 | 6 | 171  | 136  | 16  | 22 | 4 | 6                   | 215  | 12   | 44 | 16 | 8 | 6 | 585  | 598  | 19  |                     |  |  |  |  |  |  |  |  |  |
| 7                   | 7 | 5 | 480  | 488  | 9  | 7  | 11 | 5 | 98   | 58                  | 98  | 12 | 1 | 6 | 322  | 341  | 11  | 23 | 4 | 6                   | 257  | 206  | 60 | 17 | 8 | 6 | 1180 | 1195 | 13  |                     |  |  |  |  |  |  |  |  |  |
| 8                   | 7 | 5 | 434  | 433  | 15 | 8  | 11 | 5 | 219  | 232                 | 30  | 13 | 1 | 6 | 196  | 174  | 25  | 1  | 5 | 6                   | 376  | 348  | 11 | 18 | 8 | 6 | 760  | 729  | 22  |                     |  |  |  |  |  |  |  |  |  |
| 9                   | 7 | 5 | 340  | 349  | 19 | 9  | 11 | 5 | 279  | 160                 | 29  | 14 | 1 | 6 | 402  | 406  | 16  | 2  | 5 | 6                   | 1166 | 1146 | 8  | 19 | 8 | 6 | 924  | 905  | 11  |                     |  |  |  |  |  |  |  |  |  |
| 10                  | 7 | 5 | 165  | 94   | 36 | 10 | 11 | 5 | 187  | 86                  | 94  | 15 | 1 | 6 | 326  | 328  | 17  | 3  | 5 | 6                   | 729  | 724  | 8  | 20 | 8 | 6 | 402  | 407  | 22  |                     |  |  |  |  |  |  |  |  |  |
| 11                  | 7 | 5 | 433  | 443  | 15 | 11 | 11 | 5 | 259  | 314                 | 23  | 16 | 1 | 6 | 118  | 108  | 46  | 4  | 5 | 6                   | 1211 | 1196 | 7  | 21 | 8 | 6 | 802  | 858  | 30  |                     |  |  |  |  |  |  |  |  |  |
| 12                  | 7 | 5 | 622  | 622  | 10 | 12 | 11 | 5 | 163  | 77                  | 62  | 17 | 1 | 6 | 239  | 193  | 21  | 5  | 5 | 6                   | 451  | 445  | 9  | 1  | 9 | 6 | 261  | 314  | 33  |                     |  |  |  |  |  |  |  |  |  |
| 13                  | 7 | 5 | 1055 | 1049 | 11 | 13 | 11 | 5 | 539  | 540                 | 19  | 18 | 1 | 6 | 134  | 168  | 63  | 6  | 5 | 6                   | 1243 | 1249 | 15 | 2  | 9 | 6 | 889  | 889  | 19  |                     |  |  |  |  |  |  |  |  |  |
| 14                  | 7 | 5 | 728  | 741  | 11 | 14 | 11 | 5 | 287  | 272                 | 28  | 19 | 1 | 6 | 281  | 288  | 40  | 7  | 5 | 6                   | 611  | 586  | 8  | 3  | 9 | 6 | 785  | 778  | 11  |                     |  |  |  |  |  |  |  |  |  |
| 15                  | 7 | 5 | 863  | 839  | 10 | 15 | 11 | 5 | 453  | 473                 | 26  | 20 | 1 | 6 | 511  | 504  | 13  | 8  | 5 | 6                   | 247  | 209  | 20 | 4  | 9 | 6 | 1174 | 1159 | 12  |                     |  |  |  |  |  |  |  |  |  |
| 16                  | 7 | 5 | 697  | 687  | 11 | 16 | 11 | 5 | 281  | 291                 | 37  | 21 | 1 | 6 | 415  | 436  | 32  | 9  | 5 | 6                   | 287  | 255  | 23 | 5  | 9 | 6 | 569  | 573  | 17  |                     |  |  |  |  |  |  |  |  |  |
| 17                  | 7 | 5 | 556  | 597  | 29 | 17 | 11 | 5 | 473  | 530                 | 18  | 22 | 1 | 6 | 384  | 361  | 30  | 10 | 5 | 6                   | 702  | 714  | 14 | 6  | 9 | 6 | 1007 | 1010 | 11  |                     |  |  |  |  |  |  |  |  |  |
| 18                  | 7 | 5 | 196  | 2    | 48 | 18 | 11 | 5 | 156  | 3                   | 155 | 23 | 1 | 6 | 388  | 371  | 19  | 11 | 5 | 6                   | 552  | 554  | 13 | 7  | 9 | 6 | 497  | 471  | 15  |                     |  |  |  |  |  |  |  |  |  |
| 19                  | 7 | 5 | 180  | 238  | 34 | 0  | 12 | 5 | 1479 | 1509                | 18  | 24 | 1 | 6 | 692  | 676  | 26  | 12 | 5 | 6                   | 421  | 431  | 23 | 8  | 9 | 6 | 355  | 348  | 16  |                     |  |  |  |  |  |  |  |  |  |
| 20                  | 7 | 5 | 419  | 458  | 29 | 1  | 12 | 5 | 200  | 121                 | 35  | 25 | 1 | 6 | 456  | 467  | 23  | 13 | 5 | 6                   | 560  | 565  | 10 | 9  | 9 | 6 | 0    | 68   | 1   |                     |  |  |  |  |  |  |  |  |  |
| 21                  | 7 | 5 | 658  | 649  | 21 | 2  | 12 | 5 | 1198 | 1200                | 12  | 0  | 2 | 6 | 748  | 716  | 7   | 14 | 5 | 6                   | 962  | 973  | 16 | 10 | 9 | 6 | 193  | 207  | 61  |                     |  |  |  |  |  |  |  |  |  |
| 22                  | 7 | 5 | 521  | 539  | 27 | 3  | 12 | 5 | 184  | 87                  | 43  | 1  | 2 | 6 | 345  | 329  | 6   | 15 | 5 | 6                   | 280  | 224  | 28 | 11 | 9 | 6 | 90   | 210  | 90  |                     |  |  |  |  |  |  |  |  |  |
| 23                  | 7 | 5 | 844  | 826  | 26 | 4  | 12 | 5 | 642  | 613                 | 13  | 2  | 2 | 6 | 505  | 487  | 8   | 16 | 5 | 6                   | 661  | 650  | 17 | 12 | 9 | 6 | 318  | 293  | 41  |                     |  |  |  |  |  |  |  |  |  |
| 0                   | 8 | 5 | 976  | 973  | 15 | 5  | 12 | 5 | 341  | 345                 | 36  | 3  | 2 | 6 | 454  | 455  | 5   | 17 | 5 | 6                   | 177  | 121  | 46 | 13 | 9 | 6 | 327  | 324  | 16  |                     |  |  |  |  |  |  |  |  |  |
| 1                   | 8 | 5 | 613  | 610  | 11 | 6  | 12 | 5 | 269  | 165                 | 69  | 4  | 2 | 6 | 293  | 258  | 11  | 18 | 5 | 6                   | 293  | 199  | 44 | 14 | 9 | 6 | 653  | 662  | 11  |                     |  |  |  |  |  |  |  |  |  |
| 2                   | 8 | 5 | 921  | 886  | 10 | 7  | 12 | 5 | 683  | 696                 | 19  | 5  | 2 | 6 | 933  | 926  | 9   | 19 | 5 | 6                   | 190  | 128  | 44 | 15 | 9 | 6 | 155  | 51   | 52  |                     |  |  |  |  |  |  |  |  |  |
| 3                   | 8 | 5 | 234  | 199  | 25 | 8  | 12 | 5 | 104  | 123                 | 104 | 6  | 2 | 6 | 720  | 710  | 5   | 20 | 5 | 6                   | 177  | 41   | 66 | 16 |   |   |      |      |     |                     |  |  |  |  |  |  |  |  |  |



Table 6. 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 |
|----|----|---|------|------|-----|----|---|---|------|------|-----|----|---|---|------|------|-----|----|---|----|------|------|-----|----|---|----|------|------|-----|
| 16 | 7  | 8 | 64   | 103  | 64  | 17 | 1 | 9 | 56   | 10   | 56  | 4  | 6 | 9 | 554  | 541  | 22  | 9  | 0 | 10 | 1460 | 1450 | 14  | 7  | 5 | 10 | 127  | 9    | 46  |
| 17 | 7  | 8 | 191  | 206  | 44  | 18 | 1 | 9 | 275  | 149  | 275 | 5  | 6 | 9 | 139  | 79   | 40  | 10 | 0 | 10 | 341  | 359  | 26  | 8  | 5 | 10 | 305  | 333  | 17  |
| 18 | 7  | 8 | 339  | 211  | 41  | 19 | 1 | 9 | 256  | 293  | 80  | 6  | 6 | 9 | 263  | 262  | 19  | 11 | 0 | 10 | 1234 | 1238 | 17  | 9  | 5 | 10 | 91   | 44   | 90  |
| 19 | 7  | 8 | 131  | 125  | 130 | 20 | 1 | 9 | 266  | 119  | 56  | 7  | 6 | 9 | 142  | 42   | 46  | 12 | 0 | 10 | 360  | 399  | 65  | 10 | 5 | 10 | 170  | 136  | 51  |
| 0  | 8  | 8 | 926  | 913  | 17  | 0  | 2 | 9 | 2235 | 2254 | 18  | 8  | 6 | 9 | 193  | 83   | 30  | 13 | 0 | 10 | 770  | 732  | 41  | 11 | 5 | 10 | 138  | 118  | 138 |
| 1  | 8  | 8 | 513  | 509  | 11  | 1  | 2 | 9 | 167  | 109  | 23  | 9  | 6 | 9 | 248  | 77   | 73  | 14 | 0 | 10 | 369  | 400  | 42  | 12 | 5 | 10 | 662  | 693  | 25  |
| 2  | 8  | 8 | 768  | 764  | 9   | 2  | 2 | 9 | 1459 | 1451 | 10  | 10 | 6 | 9 | 162  | 128  | 124 | 15 | 0 | 10 | 0    | 101  | 1   | 13 | 5 | 10 | 0    | 105  | 1   |
| 3  | 8  | 8 | 164  | 59   | 29  | 3  | 2 | 9 | 126  | 99   | 44  | 11 | 6 | 9 | 227  | 77   | 60  | 16 | 0 | 10 | 362  | 329  | 28  | 14 | 5 | 10 | 766  | 773  | 32  |
| 4  | 8  | 8 | 582  | 567  | 21  | 4  | 2 | 9 | 761  | 740  | 14  | 12 | 6 | 9 | 266  | 125  | 24  | 17 | 0 | 10 | 701  | 720  | 34  | 15 | 5 | 10 | 254  | 217  | 39  |
| 5  | 8  | 8 | 404  | 424  | 18  | 5  | 2 | 9 | 225  | 237  | 22  | 13 | 6 | 9 | 204  | 116  | 34  | 18 | 0 | 10 | 470  | 540  | 33  | 16 | 5 | 10 | 302  | 348  | 151 |
| 6  | 8  | 8 | 244  | 153  | 27  | 6  | 2 | 9 | 231  | 205  | 22  | 14 | 6 | 9 | 208  | 249  | 24  | 1  | 1 | 10 | 0    | 102  | 1   | 0  | 6 | 10 | 386  | 396  | 36  |
| 7  | 8  | 8 | 1319 | 1298 | 15  | 7  | 2 | 9 | 146  | 25   | 32  | 15 | 6 | 9 | 153  | 59   | 59  | 2  | 1 | 10 | 266  | 271  | 19  | 1  | 6 | 10 | 1343 | 1358 | 13  |
| 8  | 8  | 8 | 455  | 439  | 19  | 8  | 2 | 9 | 390  | 393  | 19  | 16 | 6 | 9 | 364  | 338  | 55  | 3  | 1 | 10 | 183  | 11   | 65  | 2  | 6 | 10 | 344  | 336  | 18  |
| 9  | 8  | 8 | 1246 | 1226 | 12  | 9  | 2 | 9 | 142  | 36   | 43  | 17 | 6 | 9 | 229  | 15   | 65  | 4  | 1 | 10 | 697  | 714  | 10  | 3  | 6 | 10 | 607  | 603  | 14  |
| 10 | 8  | 8 | 330  | 258  | 22  | 10 | 2 | 9 | 512  | 527  | 31  | 18 | 6 | 9 | 752  | 733  | 15  | 5  | 1 | 10 | 93   | 17   | 92  | 4  | 6 | 10 | 361  | 321  | 14  |
| 11 | 8  | 8 | 625  | 600  | 15  | 11 | 2 | 9 | 251  | 241  | 31  | 1  | 7 | 9 | 230  | 294  | 25  | 6  | 1 | 10 | 443  | 459  | 23  | 5  | 6 | 10 | 154  | 133  | 38  |
| 12 | 8  | 8 | 481  | 479  | 15  | 12 | 2 | 9 | 105  | 78   | 104 | 2  | 7 | 9 | 207  | 256  | 31  | 7  | 1 | 10 | 178  | 185  | 54  | 6  | 6 | 10 | 427  | 401  | 20  |
| 13 | 8  | 8 | 502  | 506  | 18  | 13 | 2 | 9 | 108  | 27   | 107 | 3  | 7 | 9 | 745  | 735  | 15  | 8  | 1 | 10 | 233  | 254  | 32  | 7  | 6 | 10 | 239  | 267  | 39  |
| 14 | 8  | 8 | 450  | 458  | 23  | 14 | 2 | 9 | 672  | 681  | 29  | 4  | 7 | 9 | 164  | 65   | 35  | 9  | 1 | 10 | 125  | 33   | 53  | 8  | 6 | 10 | 409  | 378  | 26  |
| 15 | 8  | 8 | 189  | 59   | 60  | 15 | 2 | 9 | 127  | 77   | 46  | 5  | 7 | 9 | 784  | 779  | 11  | 10 | 1 | 10 | 106  | 182  | 67  | 9  | 6 | 10 | 563  | 570  | 21  |
| 16 | 8  | 8 | 485  | 490  | 30  | 16 | 2 | 9 | 1234 | 1252 | 17  | 6  | 7 | 9 | 199  | 50   | 45  | 11 | 1 | 10 | 156  | 130  | 83  | 10 | 6 | 10 | 438  | 460  | 33  |
| 17 | 8  | 8 | 483  | 489  | 19  | 17 | 2 | 9 | 259  | 107  | 32  | 7  | 7 | 9 | 643  | 635  | 13  | 12 | 1 | 10 | 438  | 447  | 43  | 11 | 6 | 10 | 451  | 437  | 35  |
| 18 | 8  | 8 | 482  | 476  | 23  | 18 | 2 | 9 | 905  | 930  | 18  | 8  | 7 | 9 | 242  | 29   | 39  | 13 | 1 | 10 | 175  | 89   | 63  | 12 | 6 | 10 | 416  | 445  | 32  |
| 1  | 9  | 8 | 127  | 151  | 58  | 19 | 2 | 9 | 233  | 32   | 183 | 9  | 7 | 9 | 277  | 217  | 22  | 14 | 1 | 10 | 495  | 505  | 25  | 13 | 6 | 10 | 190  | 151  | 87  |
| 2  | 9  | 8 | 694  | 684  | 13  | 20 | 2 | 9 | 1007 | 990  | 27  | 10 | 7 | 9 | 186  | 124  | 51  | 15 | 1 | 10 | 320  | 105  | 43  | 14 | 6 | 10 | 221  | 228  | 156 |
| 3  | 9  | 8 | 58   | 77   | 58  | 1  | 3 | 9 | 226  | 214  | 18  | 11 | 7 | 9 | 668  | 662  | 53  | 16 | 1 | 10 | 339  | 271  | 28  | 15 | 6 | 10 | 777  | 778  | 36  |
| 4  | 9  | 8 | 888  | 879  | 16  | 2  | 3 | 9 | 19   | 58   | 18  | 12 | 7 | 9 | 242  | 78   | 26  | 17 | 1 | 10 | 258  | 66   | 38  | 1  | 7 | 10 | 114  | 25   | 114 |
| 5  | 9  | 8 | 186  | 198  | 62  | 3  | 3 | 9 | 91   | 3    | 61  | 13 | 7 | 9 | 1096 | 1109 | 12  | 18 | 1 | 10 | 281  | 193  | 141 | 2  | 7 | 10 | 86   | 18   | 85  |
| 6  | 9  | 8 | 897  | 892  | 10  | 4  | 3 | 9 | 105  | 123  | 62  | 14 | 7 | 9 | 195  | 110  | 48  | 0  | 2 | 10 | 218  | 319  | 35  | 3  | 7 | 10 | 178  | 24   | 68  |
| 7  | 9  | 8 | 0    | 21   | 1   | 5  | 3 | 9 | 158  | 158  | 37  | 15 | 7 | 9 | 769  | 813  | 15  | 1  | 2 | 10 | 985  | 1008 | 19  | 4  | 7 | 10 | 42   | 143  | 41  |
| 8  | 9  | 8 | 215  | 139  | 27  | 6  | 3 | 9 | 171  | 145  | 46  | 16 | 7 | 9 | 119  | 84   | 66  | 2  | 2 | 10 | 293  | 310  | 18  | 5  | 7 | 10 | 99   | 93   | 98  |
| 9  | 9  | 8 | 189  | 36   | 52  | 7  | 3 | 9 | 126  | 135  | 47  | 17 | 7 | 9 | 517  | 553  | 29  | 3  | 2 | 10 | 652  | 652  | 11  | 6  | 7 | 10 | 98   | 29   | 97  |
| 10 | 9  | 8 | 648  | 664  | 31  | 8  | 3 | 9 | 138  | 25   | 29  | 0  | 8 | 9 | 178  | 73   | 45  | 4  | 2 | 10 | 292  | 308  | 17  | 7  | 7 | 10 | 107  | 109  | 107 |
| 11 | 9  | 8 | 263  | 231  | 24  | 9  | 3 | 9 | 116  | 21   | 66  | 1  | 8 | 9 | 128  | 121  | 37  | 5  | 2 | 10 | 68   | 38   | 67  | 8  | 7 | 10 | 213  | 44   | 44  |
| 12 | 9  | 8 | 747  | 738  | 21  | 10 | 3 | 9 | 174  | 8    | 60  | 2  | 8 | 9 | 217  | 169  | 43  | 6  | 2 | 10 | 172  | 221  | 29  | 9  | 7 | 10 | 194  | 230  | 32  |
| 13 | 9  | 8 | 299  | 128  | 37  | 11 | 3 | 9 | 394  | 443  | 21  | 3  | 8 | 9 | 184  | 76   | 62  | 7  | 2 | 10 | 190  | 202  | 47  | 10 | 7 | 10 | 272  | 39   | 44  |
| 14 | 9  | 8 | 893  | 907  | 17  | 12 | 3 | 9 | 180  | 115  | 42  | 4  | 8 | 9 | 287  | 291  | 29  | 8  | 2 | 10 | 367  | 377  | 15  | 11 | 7 | 10 | 197  | 158  | 39  |
| 15 | 9  | 8 | 244  | 191  | 44  | 13 | 3 | 9 | 664  | 671  | 17  | 5  | 8 | 9 | 109  | 115  | 81  | 9  | 2 | 10 | 325  | 364  | 31  | 12 | 7 | 10 | 279  | 170  | 59  |
| 16 | 9  | 8 | 415  | 517  | 47  | 14 | 3 | 9 | 169  | 153  | 84  | 6  | 8 | 9 | 548  | 551  | 11  | 10 | 2 | 10 | 378  | 348  | 28  | 13 | 7 | 10 | 112  | 111  | 111 |
| 0  | 10 | 8 | 102  | 157  | 102 | 15 | 3 | 9 | 459  | 433  | 15  | 7  | 8 | 9 | 280  | 20   | 65  | 11 | 2 | 10 | 293  | 211  | 19  | 0  | 8 | 10 | 677  | 656  | 20  |
| 1  | 10 | 8 | 59   | 36   | 59  | 16 | 3 | 9 | 184  | 100  | 48  | 8  | 8 | 9 | 692  | 674  | 18  | 12 | 2 | 10 | 343  | 355  | 48  | 1  | 8 | 10 | 430  | 448  | 17  |
| 2  | 10 | 8 | 0    | 176  | 1   | 17 | 3 | 9 | 551  | 539  | 16  | 9  | 8 | 9 | 219  | 35   | 24  | 13 | 2 | 10 | 271  | 250  | 46  | 2  | 8 | 10 | 356  | 379  | 19  |
| 3  | 10 | 8 | 230  | 192  | 30  | 18 | 3 | 9 | 145  | 162  | 144 | 10 | 8 | 9 | 669  | 660  | 13  | 14 | 2 | 10 | 220  | 284  | 41  | 3  | 8 | 10 | 211  | 28   | 34  |
| 4  | 10 | 8 | 228  | 42   | 34  | 19 | 3 | 9 | 87   | 81   | 87  | 11 | 8 | 9 | 129  | 5    | 128 | 15 | 2 | 10 | 711  | 720  | 22  | 4  | 8 | 10 | 351  | 322  | 29  |
| 5  | 10 | 8 | 244  | 224  | 54  | 20 | 3 | 9 | 108  | 73   | 107 | 12 | 8 | 9 | 585  | 601  | 31  | 16 | 2 | 10 | 204  | 170  | 30  | 5  | 8 | 10 | 531  | 536  | 14  |
| 6  | 10 | 8 | 67   | 45   | 66  | 0  | 4 | 9 | 519  | 465  | 14  | 13 | 8 | 9 | 208  | 10   | 43  | 17 | 2 | 10 | 621  | 668  | 18  | 6  | 8 | 10 | 324  | 273  | 18  |
| 7  | 10 | 8 | 316  | 325  | 43  | 1  | 4 | 9 | 190  | 179  | 21  | 14 | 8 | 9 | 121  | 101  | 73  | 18 | 2 | 10 | 299  | 109  | 47  | 7  | 8 | 10 | 896  | 905  | 14  |
| 8  | 10 | 8 | 272  | 276  | 75  | 2  | 4 | 9 | 210  | 82   | 49  | 15 | 8 | 9 | 196  | 76   | 51  | 1  | 3 | 10 | 149  | 52   | 38  | 8  | 8 | 10 | 357  | 293  | 45  |
| 9  | 10 | 8 | 157  | 38   | 42  | 3  | 4 | 9 | 201  | 133  | 24  | 1  | 9 | 9 | 101  | 17   | 101 | 2  | 3 | 10 | 770  | 779  | 11  | 9  | 8 | 10 | 1095 | 1061 | 21  |
| 10 | 10 | 8 | 276  | 207  | 31  | 4  | 4 | 9 | 614  | 607  | 9   | 2  | 9 | 9 | 204  | 90   | 58  | 3  | 3 | 10 | 238  | 52   | 40  | 10 | 8 | 10 | 326  | 262  | 77  |
| 11 | 10 | 8 | 90   | 44   | 90  | 5  | 4 | 9 | 79   | 98   | 79  | 3  | 9 | 9 | 659  | 648  | 11  | 4  | 3 | 10 | 1040 | 1062 | 12  | 11 | 8 | 10 | 968  | 976  | 26  |
| 12 | 10 | 8 | 283  | 236  | 35  | 6  | 4 | 9 | 1458 | 1481 | 15  | 4  | 9 | 9 | 197  | 67   | 37  | 5  | 3 | 10 | 148  | 81   | 46  | 12 | 8 | 10 | 372  | 288  | 41  |
| 13 | 10 | 8 | 136  | 96   | 136 | 7  | 4 | 9 | 160  | 69   | 30  | 5  | 9 | 9 | 661  | 654  | 12  | 6  | 3 | 10 | 1118 | 1102 | 10  | 1  | 9 | 10 | 261  | 31   | 59  |
| 14 | 10 | 8 | 318  | 304  | 52  | 8  | 4 | 9 | 1762 | 1763 | 12  | 6  | 9 | 9 | 267  | 108  | 55  | 7  | 3 | 10 | 46   | 96   | 46  | 2  | 9 | 10 | 712  | 758  | 16  |
| 2  | 11 | 8 | 564  | 557  | 15  | 9  | 4 | 9 | 217  | 61   | 26  | 7  | 9 | 9 | 380  | 366  | 20  | 8  | 3 | 10 | 549  | 580  | 11  | 3  | 9 | 10 | 106  | 18   | 105 |
| 3  | 11 | 8 | 150  | 129  | 62  | 10 | 4 | 9 | 1790 | 1805 | 12  | 8  | 9 | 9 | 210  | 52   | 46  | 9  | 3 | 10 | 185  | 146  | 115 | 4  | 9 | 10 | 755  | 760  | 21  |
| 4  | 11 | 8 | 842  | 847  | 13  | 11 | 4 | 9 | 2    |      |     |    |   |   |      |      |     |    |   |    |      |      |     |    |   |    |      |      |     |

Table 6. 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 |
|----|---|----|------|------|-----|----|---|----|------|------|-----|----|---|----|------|------|-----|---|---|----|------|------|-----|---|---|----|------|------|-----|
| 8  | 2 | 11 | 475  | 504  | 13  | 4  | 4 | 11 | 393  | 370  | 21  | 3  | 6 | 11 | 222  | 123  | 27  | 2 | 0 | 12 | 638  | 613  | 41  | 1 | 3 | 12 | 199  | 220  | 54  |
| 9  | 2 | 11 | 622  | 601  | 23  | 5  | 4 | 11 | 569  | 570  | 12  | 4  | 6 | 11 | 163  | 191  | 34  | 3 | 0 | 12 | 754  | 761  | 18  | 2 | 3 | 12 | 726  | 769  | 22  |
| 10 | 2 | 11 | 859  | 874  | 14  | 6  | 4 | 11 | 318  | 359  | 34  | 5  | 6 | 11 | 217  | 174  | 75  | 4 | 0 | 12 | 491  | 502  | 28  | 3 | 3 | 12 | 220  | 291  | 49  |
| 11 | 2 | 11 | 742  | 741  | 15  | 7  | 4 | 11 | 257  | 267  | 56  | 6  | 6 | 11 | 130  | 212  | 129 | 5 | 0 | 12 | 0    | 249  | 1   | 4 | 3 | 12 | 897  | 926  | 24  |
| 12 | 2 | 11 | 566  | 617  | 46  | 8  | 4 | 11 | 904  | 920  | 15  | 7  | 6 | 11 | 393  | 343  | 44  | 6 | 0 | 12 | 209  | 219  | 67  | 5 | 3 | 12 | 385  | 372  | 18  |
| 13 | 2 | 11 | 391  | 407  | 31  | 9  | 4 | 11 | 159  | 305  | 159 | 8  | 6 | 11 | 483  | 483  | 31  | 7 | 0 | 12 | 370  | 360  | 29  | 6 | 3 | 12 | 850  | 872  | 13  |
| 14 | 2 | 11 | 137  | 134  | 137 | 10 | 4 | 11 | 963  | 1007 | 17  | 9  | 6 | 11 | 416  | 347  | 34  | 8 | 0 | 12 | 197  | 267  | 81  | 7 | 3 | 12 | 475  | 406  | 25  |
| 15 | 2 | 11 | 286  | 228  | 34  | 11 | 4 | 11 | 278  | 356  | 27  | 10 | 6 | 11 | 283  | 227  | 55  | 9 | 0 | 12 | 354  | 431  | 41  | 9 | 3 | 12 | 0    | 3    | 1   |
| 1  | 3 | 11 | 0    | 5    | 1   | 12 | 4 | 11 | 659  | 638  | 56  | 1  | 7 | 11 | 398  | 348  | 27  | 1 | 1 | 12 | 174  | 38   | 49  | 0 | 4 | 12 | 225  | 130  | 60  |
| 2  | 3 | 11 | 0    | 92   | 1   | 13 | 4 | 11 | 368  | 418  | 23  | 2  | 7 | 11 | 300  | 229  | 32  | 2 | 1 | 12 | 278  | 287  | 63  | 1 | 4 | 12 | 333  | 368  | 56  |
| 3  | 3 | 11 | 221  | 204  | 29  | 1  | 5 | 11 | 288  | 281  | 53  | 3  | 7 | 11 | 729  | 714  | 12  | 3 | 1 | 12 | 202  | 238  | 44  | 2 | 4 | 12 | 290  | 181  | 32  |
| 4  | 3 | 11 | 138  | 100  | 52  | 2  | 5 | 11 | 0    | 128  | 1   | 4  | 7 | 11 | 359  | 270  | 51  | 4 | 1 | 12 | 446  | 501  | 25  | 3 | 4 | 12 | 214  | 194  | 50  |
| 5  | 3 | 11 | 342  | 283  | 18  | 3  | 5 | 11 | 759  | 754  | 27  | 5  | 7 | 11 | 923  | 944  | 18  | 5 | 1 | 12 | 184  | 163  | 52  | 4 | 4 | 12 | 259  | 69   | 138 |
| 6  | 3 | 11 | 209  | 193  | 50  | 4  | 5 | 11 | 252  | 164  | 49  | 6  | 7 | 11 | 361  | 316  | 31  | 6 | 1 | 12 | 492  | 465  | 22  | 5 | 4 | 12 | 192  | 24   | 76  |
| 7  | 3 | 11 | 86   | 114  | 86  | 5  | 5 | 11 | 605  | 589  | 18  | 7  | 7 | 11 | 579  | 580  | 41  | 7 | 1 | 12 | 300  | 165  | 39  | 6 | 4 | 12 | 143  | 10   | 124 |
| 8  | 3 | 11 | 290  | 278  | 50  | 6  | 5 | 11 | 236  | 119  | 35  | 8  | 7 | 11 | 190  | 121  | 53  | 8 | 1 | 12 | 190  | 271  | 189 | 7 | 4 | 12 | 171  | 110  | 120 |
| 9  | 3 | 11 | 161  | 127  | 59  | 7  | 5 | 11 | 451  | 424  | 32  | 0  | 8 | 11 | 398  | 403  | 42  | 0 | 2 | 12 | 64   | 99   | 64  | 8 | 4 | 12 | 0    | 186  | 1   |
| 10 | 3 | 11 | 176  | 137  | 52  | 8  | 5 | 11 | 217  | 212  | 34  | 1  | 8 | 11 | 268  | 172  | 54  | 1 | 2 | 12 | 227  | 141  | 56  | 2 | 5 | 12 | 423  | 338  | 61  |
| 11 | 3 | 11 | 113  | 8    | 113 | 9  | 5 | 11 | 239  | 246  | 31  | 2  | 8 | 11 | 492  | 429  | 39  | 2 | 2 | 12 | 175  | 153  | 42  | 3 | 5 | 12 | 342  | 240  | 79  |
| 12 | 3 | 11 | 228  | 242  | 39  | 10 | 5 | 11 | 170  | 150  | 43  | 3  | 8 | 11 | 392  | 358  | 32  | 3 | 2 | 12 | 219  | 23   | 218 | 4 | 5 | 12 | 618  | 616  | 20  |
| 14 | 3 | 11 | 175  | 217  | 82  | 11 | 5 | 11 | 122  | 210  | 122 | 4  | 8 | 11 | 145  | 142  | 66  | 4 | 2 | 12 | 217  | 131  | 80  | 5 | 5 | 12 | 418  | 299  | 30  |
| 0  | 4 | 11 | 1150 | 1164 | 17  | 12 | 5 | 11 | 208  | 11   | 78  | 5  | 8 | 11 | 335  | 227  | 26  | 5 | 2 | 12 | 328  | 344  | 62  | 6 | 5 | 12 | 462  | 452  | 29  |
| 1  | 4 | 11 | 811  | 808  | 12  | 0  | 6 | 11 | 340  | 221  | 24  | 6  | 8 | 11 | 232  | 160  | 60  | 6 | 2 | 12 | 302  | 298  | 26  |   |   |    |      |      |     |
| 2  | 4 | 11 | 857  | 849  | 15  | 1  | 6 | 11 | 310  | 322  | 42  | 0  | 0 | 12 | 890  | 875  | 24  | 7 | 2 | 12 | 517  | 523  | 15  |   |   |    |      |      |     |
| 3  | 4 | 11 | 776  | 797  | 14  | 2  | 6 | 11 | 386  | 353  | 16  | 1  | 0 | 12 | 1462 | 1470 | 22  | 8 | 2 | 12 | 303  | 360  | 45  |   |   |    |      |      |     |

Table 6. Observed and calculated structure factors for 1

Page 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 |
|----|---|-----|------|------|-----|----|---|----|------|------|-----|----|---|----|------|------|-----|----|----|----|------|------|-----|----|---|----|------|------|-----|
| 5  | 0 | -11 | 194  | 193  | 3   | 7  | 3 | -9 | 117  | 119  | 3   | 6  | 5 | -8 | 173  | 174  | 5   | 1  | 5  | -7 | 206  | 206  | 4   | 1  | 3 | -6 | 256  | 249  | 2   |
| 2  | 1 | -11 | 62   | 55   | 4   | -1 | 4 | -9 | 259  | 238  | 4   | 7  | 5 | -8 | 123  | 119  | 3   | 2  | 5  | -7 | 170  | 164  | 2   | 2  | 3 | -6 | 267  | 264  | 3   |
| 3  | 1 | -11 | 159  | 165  | 6   | 0  | 4 | -9 | 145  | 145  | 3   | -3 | 6 | -8 | 135  | 133  | 5   | 3  | 5  | -7 | 106  | 108  | 2   | 3  | 3 | -6 | 86   | 75   | 3   |
| 5  | 1 | -11 | 162  | 164  | 3   | 1  | 4 | -9 | 177  | 176  | 4   | -2 | 6 | -8 | 162  | 156  | 2   | 4  | 5  | -7 | 363  | 368  | 9   | 4  | 3 | -6 | 363  | 365  | 7   |
| 1  | 2 | -11 | 183  | 185  | 2   | 2  | 4 | -9 | 191  | 189  | 2   | -1 | 6 | -8 | 168  | 160  | 5   | 5  | 5  | -7 | 143  | 144  | 2   | 5  | 3 | -6 | 165  | 159  | 7   |
| 2  | 2 | -11 | 78   | 78   | 4   | 3  | 4 | -9 | 189  | 187  | 2   | 0  | 6 | -8 | 189  | 189  | 2   | 6  | 5  | -7 | 171  | 164  | 3   | 6  | 3 | -6 | 210  | 212  | 3   |
| 3  | 2 | -11 | 153  | 157  | 3   | 4  | 4 | -9 | 87   | 100  | 3   | 1  | 6 | -8 | 200  | 201  | 4   | 7  | 5  | -7 | 114  | 111  | 3   | 7  | 3 | -6 | 92   | 95   | 2   |
| 4  | 2 | -11 | 81   | 84   | 4   | 5  | 4 | -9 | 156  | 160  | 2   | 2  | 6 | -8 | 133  | 131  | 2   | -4 | 6  | -7 | 236  | 212  | 3   | 8  | 3 | -6 | 45   | 44   | 3   |
| 0  | 3 | -11 | 151  | 148  | 2   | 6  | 4 | -9 | 122  | 119  | 9   | 3  | 6 | -8 | 132  | 134  | 2   | -3 | 6  | -7 | 235  | 234  | 5   | -4 | 4 | -6 | 232  | 222  | 3   |
| 1  | 3 | -11 | 283  | 279  | 6   | -2 | 5 | -9 | 83   | 88   | 2   | 4  | 6 | -8 | 156  | 154  | 2   | -2 | 6  | -7 | 358  | 349  | 8   | -3 | 4 | -6 | 147  | 136  | 2   |
| 2  | 3 | -11 | 154  | 150  | 2   | -1 | 5 | -9 | 158  | 148  | 4   | 5  | 6 | -8 | 127  | 125  | 2   | -1 | 6  | -7 | 364  | 359  | 3   | -2 | 4 | -6 | 144  | 123  | 2   |
| 3  | 3 | -11 | 156  | 155  | 3   | 0  | 5 | -9 | 124  | 116  | 4   | 6  | 6 | -8 | 176  | 187  | 3   | 0  | 6  | -7 | 255  | 243  | 2   | 0  | 4 | -6 | 165  | 169  | 2   |
| 4  | 3 | -11 | 123  | 124  | 2   | 1  | 5 | -9 | 124  | 117  | 2   | -4 | 7 | -8 | 200  | 193  | 4   | 1  | 6  | -7 | 351  | 352  | 2   | 1  | 4 | -6 | 82   | 73   | 1   |
| 0  | 4 | -11 | 192  | 196  | 3   | 2  | 5 | -9 | 250  | 248  | 2   | -3 | 7 | -8 | 237  | 227  | 5   | 2  | 6  | -7 | 265  | 264  | 2   | 2  | 4 | -6 | 258  | 259  | 3   |
| 1  | 4 | -11 | 202  | 204  | 5   | 3  | 5 | -9 | 139  | 134  | 2   | -2 | 7 | -8 | 118  | 113  | 8   | 3  | 6  | -7 | 266  | 269  | 3   | 3  | 4 | -6 | 105  | 103  | 3   |
| 2  | 4 | -11 | 8    | 9    | 7   | 4  | 5 | -9 | 69   | 67   | 2   | -1 | 7 | -8 | 197  | 192  | 2   | 4  | 6  | -7 | 198  | 205  | 2   | 4  | 4 | -6 | 169  | 171  | 5   |
| 3  | 4 | -11 | 164  | 160  | 3   | 5  | 5 | -9 | 129  | 129  | 8   | 0  | 7 | -8 | 252  | 254  | 5   | 5  | 6  | -7 | 256  | 265  | 2   | 5  | 4 | -6 | 117  | 117  | 1   |
| 0  | 5 | -11 | 193  | 182  | 3   | -3 | 6 | -9 | 167  | 169  | 3   | 1  | 7 | -8 | 139  | 135  | 6   | 6  | 6  | -7 | 99   | 100  | 4   | 6  | 4 | -6 | 351  | 340  | 7   |
| 1  | 5 | -11 | 127  | 130  | 2   | -2 | 6 | -9 | 162  | 162  | 3   | 2  | 7 | -8 | 67   | 68   | 2   | 7  | 6  | -7 | 98   | 103  | 5   | 7  | 4 | -6 | 64   | 60   | 2   |
| 2  | 5 | -11 | 87   | 84   | 8   | -1 | 6 | -9 | 104  | 99   | 4   | 3  | 7 | -8 | 188  | 186  | 3   | -5 | 7  | -7 | 86   | 90   | 3   | 8  | 4 | -6 | 154  | 154  | 3   |
| 4  | 0 | -10 | 255  | 251  | 4   | 0  | 6 | -9 | 167  | 157  | 3   | 4  | 7 | -8 | 96   | 92   | 4   | -4 | 7  | -7 | 174  | 163  | 3   | -4 | 5 | -6 | 293  | 280  | 4   |
| 6  | 0 | -10 | 78   | 76   | 4   | 1  | 6 | -9 | 205  | 198  | 2   | 5  | 7 | -8 | 83   | 91   | 2   | -3 | 7  | -7 | 169  | 159  | 3   | -3 | 5 | -6 | 390  | 369  | 5   |
| 1  | 1 | -10 | 167  | 165  | 3   | 2  | 6 | -9 | 208  | 206  | 5   | -2 | 8 | -8 | 215  | 184  | 4   | -2 | 7  | -7 | 167  | 162  | 3   | -2 | 5 | -6 | 283  | 273  | 4   |
| 2  | 1 | -10 | 230  | 224  | 3   | 3  | 6 | -9 | 151  | 149  | 3   | -3 | 8 | -8 | 56   | 46   | 4   | -1 | 7  | -7 | 233  | 226  | 2   | -1 | 5 | -6 | 198  | 193  | 3   |
| 3  | 1 | -10 | 69   | 69   | 3   | 4  | 6 | -9 | 74   | 79   | 7   | -1 | 8 | -8 | 155  | 155  | 2   | 0  | 7  | -7 | 186  | 184  | 3   | 0  | 5 | -6 | 445  | 443  | 5   |
| 4  | 1 | -10 | 217  | 211  | 3   | 5  | 6 | -9 | 139  | 152  | 2   | 0  | 8 | -8 | 74   | 79   | 2   | 1  | 7  | -7 | 57   | 63   | 2   | 1  | 5 | -6 | 297  | 294  | 2   |
| 5  | 1 | -10 | 127  | 132  | 7   | -2 | 7 | -9 | 147  | 148  | 7   | 1  | 8 | -8 | 99   | 98   | 2   | 2  | 7  | -7 | 263  | 265  | 2   | 2  | 5 | -6 | 318  | 316  | 4   |
| 6  | 1 | -10 | 105  | 108  | 3   | -1 | 7 | -9 | 80   | 73   | 2   | 2  | 8 | -8 | 47   | 45   | 3   | 3  | 7  | -7 | 111  | 114  | 2   | 3  | 5 | -6 | 411  | 407  | 9   |
| 1  | 2 | -10 | 121  | 114  | 1   | 0  | 7 | -9 | 113  | 115  | 3   | 3  | 8 | -8 | 169  | 172  | 2   | 4  | 7  | -7 | 151  | 142  | 2   | 4  | 5 | -6 | 284  | 284  | 6   |
| 2  | 2 | -10 | 160  | 165  | 3   | 1  | 7 | -9 | 133  | 133  | 2   | 4  | 8 | -8 | 68   | 66   | 8   | 5  | 7  | -7 | 171  | 185  | 2   | 5  | 5 | -6 | 113  | 117  | 4   |
| 3  | 2 | -10 | 41   | 29   | 3   | 2  | 7 | -9 | 40   | 57   | 4   | 5  | 8 | -8 | 107  | 103  | 3   | 6  | 7  | -7 | 209  | 211  | 3   | 6  | 5 | -6 | 194  | 195  | 3   |
| 4  | 2 | -10 | 153  | 152  | 3   | 3  | 7 | -9 | 132  | 124  | 3   | -1 | 9 | -8 | 217  | 208  | 5   | -4 | 8  | -7 | 187  | 182  | 3   | 7  | 5 | -6 | 171  | 179  | 10  |
| 5  | 2 | -10 | 122  | 119  | 4   | 4  | 7 | -9 | 131  | 143  | 2   | 0  | 9 | -8 | 28   | 32   | 6   | -3 | 8  | -7 | 105  | 101  | 3   | 8  | 5 | -6 | 77   | 85   | 4   |
| 6  | 2 | -10 | 213  | 205  | 3   | -1 | 8 | -9 | 38   | 25   | 6   | 1  | 9 | -8 | 228  | 214  | 2   | -2 | 8  | -7 | 167  | 166  | 5   | -4 | 6 | -6 | 72   | 55   | 3   |
| 0  | 3 | -10 | 356  | 364  | 11  | 0  | 8 | -9 | 209  | 216  | 4   | 2  | 9 | -8 | 148  | 150  | 4   | -1 | 8  | -7 | 109  | 107  | 2   | -3 | 6 | -6 | 265  | 256  | 5   |
| 1  | 3 | -10 | 95   | 97   | 2   | 1  | 8 | -9 | 83   | 72   | 8   | 3  | 9 | -8 | 242  | 236  | 4   | 0  | 8  | -7 | 226  | 217  | 2   | -2 | 6 | -6 | 100  | 105  | 2   |
| 2  | 3 | -10 | 215  | 223  | 3   | 2  | 8 | -9 | 115  | 110  | 2   | -1 | 0 | -7 | 706  | 680  | 9   | 1  | 8  | -7 | 98   | 95   | 9   | -1 | 6 | -6 | 148  | 145  | 2   |
| 3  | 3 | -10 | 26   | 26   | 10  | 3  | 8 | -9 | 33   | 33   | 8   | 3  | 0 | -7 | 457  | 465  | 6   | 2  | 8  | -7 | 255  | 256  | 2   | 0  | 6 | -6 | 128  | 129  | 2   |
| 4  | 3 | -10 | 181  | 185  | 2   | 0  | 0 | -8 | 555  | 523  | 7   | 5  | 0 | -7 | 390  | 399  | 5   | 3  | 8  | -7 | 118  | 116  | 2   | 1  | 6 | -6 | 215  | 204  | 2   |
| 5  | 3 | -10 | 87   | 89   | 3   | 2  | 0 | -8 | 214  | 228  | 3   | 7  | 0 | -7 | 157  | 156  | 3   | 4  | 8  | -7 | 87   | 85   | 2   | 2  | 6 | -6 | 169  | 174  | 5   |
| -1 | 4 | -10 | 134  | 133  | 2   | 4  | 0 | -8 | 291  | 295  | 4   | -1 | 1 | -7 | 555  | 525  | 7   | 5  | 8  | -7 | 159  | 157  | 3   | 3  | 6 | -6 | 258  | 257  | 2   |
| 0  | 4 | -10 | 267  | 258  | 2   | 6  | 0 | -8 | 404  | 401  | 5   | 0  | 1 | -7 | 196  | 192  | 3   | 6  | 8  | -7 | 226  | 226  | 10  | 4  | 6 | -6 | 221  | 225  | 6   |
| 1  | 4 | -10 | 62   | 58   | 4   | 0  | 1 | -8 | 565  | 563  | 7   | 1  | 1 | -7 | 277  | 285  | 3   | -3 | 9  | -7 | 101  | 98   | 5   | 5  | 6 | -6 | 153  | 152  | 3   |
| 2  | 4 | -10 | 184  | 190  | 5   | 1  | 1 | -8 | 157  | 152  | 2   | 2  | 1 | -7 | 169  | 164  | 3   | -2 | 9  | -7 | 141  | 149  | 2   | 6  | 6 | -6 | 146  | 155  | 6   |
| 3  | 4 | -10 | 162  | 160  | 2   | 2  | 1 | -8 | 261  | 266  | 2   | 3  | 1 | -7 | 381  | 379  | 3   | -1 | 9  | -7 | 82   | 76   | 4   | 7  | 6 | -6 | 209  | 217  | 3   |
| 4  | 4 | -10 | 212  | 219  | 2   | 3  | 1 | -8 | 82   | 80   | 2   | 4  | 1 | -7 | 80   | 89   | 1   | 0  | 9  | -7 | 157  | 153  | 2   | -5 | 7 | -6 | 149  | 157  | 5   |
| 5  | 4 | -10 | 55   | 57   | 4   | 4  | 1 | -8 | 391  | 392  | 5   | 5  | 1 | -7 | 347  | 336  | 4   | 1  | 9  | -7 | 116  | 116  | 7   | -4 | 7 | -6 | 163  | 150  | 4   |
| -2 | 5 | -10 | 100  | 99   | 3   | 5  | 1 | -8 | 80   | 82   | 7   | 6  | 1 | -7 | 146  | 145  | 5   | 2  | 9  | -7 | 215  | 222  | 5   | -3 | 7 | -6 | 169  | 179  | 3   |
| -1 | 5 | -10 | 184  | 188  | 4   | 6  | 1 | -8 | 247  | 248  | 2   | 7  | 1 | -7 | 191  | 189  | 2   | 3  | 9  | -7 | 42   | 33   | 11  | -2 | 7 | -6 | 176  | 169  | 1   |
| 0  | 5 | -10 | 89   | 82   | 2   | 7  | 1 | -8 | 106  | 104  | 3   | 8  | 1 | -7 | 81   | 87   | 2   | 4  | 9  | -7 | 101  | 108  | 2   | -1 | 7 | -6 | 220  | 227  | 2   |
| 1  | 5 | -10 | 35   | 39   | 3   | -1 | 2 | -8 | 42   | 38   | 3   | -2 | 2 | -7 | 238  | 230  | 3   | 5  | 9  | -7 | 36   | 21   | 8   | 0  | 7 | -6 | 87   | 86   | 4   |
| 2  | 5 | -10 | 76   | 74   | 2   | 0  | 2 | -8 | 82   | 83   | 2   | -1 | 2 | -7 | 353  | 332  | 4   | -1 | 10 | -7 | 113  | 104  | 3   | 1  | 7 | -6 | 337  | 340  | 3   |
| 3  | 5 | -10 | 229  | 235  | 4   | 1  | 2 | -8 | 292  | 286  | 4   | 0  | 2 | -7 | 143  | 138  | 2   | 0  | 10 | -7 | 143  | 151  | 2   | 2  | 7 | -6 | 225  | 233  | 2   |
| 4  | 5 | -10 | 47   | 50   | 7   | 2  | 2 | -8 | 213  | 223  | 1   | 1  | 2 | -7 | 386  | 376  | 5   | 1  | 10 | -7 | 116  | 122  | 2   | 3  | 7 | -6 | 208  | 216  | 2   |
| -1 | 6 | -10 | 107  | 113  | 3   | 3  | 2 | -8 | 135  | 135  | 1   | 2  | 2 | -7 | 330  | 333  | 2   | 2  | 10 | -7 | 149  | 148  | 2   | 4  | 7 | -6 | 106  | 109  | 3   |
| 0  | 6 | -10 | 87   | 88   | 2   | 4  | 2 | -8 | 205  | 209  | 2   | 3  | 2 | -7 | 341  | 333  | 5   | 3  | 10 | -7 | 87   | 88   | 4   | 5  | 7 | -6 | 256  | 258  | 4   |
| 1  | 6 | -10 | 73   | 66   | 2   | 5  | 2 | -8 | 129  | 136  | 2   | 4  | 2 | -7 | 93   | 93   | 2   | -2 | 0  | -6 | 481  | 467  | 6   | 6  | 7 | -6 | 139  | 150  | 2   |
| 2  | 6 | -10 | 129  | 132  | 2   | 6  | 2 | -8 | 140  | 134  | 4   | 5  | 2 | -7 | 157  | 154  | 3   | 0  | 0  | -6 | 123  | 121  | 2   | 7  | 7 | -6 | 175  | 184  | 4   |
| 3  | 6 | -10 | 122  | 131  | 3   | 7  | 2 | -8 | 92   | 92   | 3   | 6  | 2 | -7 | 266  | 258  | 6   | 2  | 0  | -6 | 463  | 474  | 6   | -5 | 8 | -6 |      |      |     |

Table 6. 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 |     |     |   |  |
|---------------------|-----|-----|----|--|---------------------|-----|-----|----|--|---------------------|-----|-----|----|--|---------------------|-----|-----|----|--|---------------------|-----|-----|---|--|
| -1 11 -6            | 194 | 197 | 3  |  | -3 7 -5             | 180 | 180 | 1  |  | 3 3 -4              | 291 | 281 | 12 |  | -2 11 -4            | 60  | 53  | 12 |  | 5 6 -3              | 203 | 208 | 4 |  |
| 0 11 -6             | 57  | 39  | 5  |  | -2 7 -5             | 139 | 129 | 2  |  | 4 3 -4              | 278 | 284 | 5  |  | -1 11 -4            | 168 | 171 | 3  |  | 6 6 -3              | 131 | 126 | 2 |  |
| 1 11 -6             | 145 | 144 | 3  |  | -1 7 -5             | 123 | 135 | 2  |  | 5 3 -4              | 110 | 108 | 5  |  | 0 11 -4             | 48  | 48  | 5  |  | 7 6 -3              | 80  | 84  | 4 |  |
| 2 11 -6             | 83  | 88  | 4  |  | 0 7 -5              | 180 | 163 | 1  |  | 6 3 -4              | 255 | 255 | 2  |  | 1 11 -4             | 156 | 163 | 4  |  | 8 6 -3              | 149 | 143 | 3 |  |
| -1 0 -5             | 171 | 143 | 2  |  | 1 7 -5              | 279 | 270 | 4  |  | 7 3 -4              | 117 | 115 | 2  |  | 2 11 -4             | 61  | 61  | 3  |  | -4 7 -3             | 225 | 219 | 2 |  |
| 3 0 -5              | 319 | 324 | 3  |  | 2 7 -5              | 128 | 126 | 2  |  | 8 3 -4              | 269 | 267 | 4  |  | 3 11 -4             | 114 | 111 | 5  |  | -3 7 -3             | 102 | 90  | 1 |  |
| 5 0 -5              | 101 | 104 | 2  |  | 3 7 -5              | 207 | 226 | 2  |  | 9 3 -4              | 95  | 100 | 3  |  | -2 12 -4            | 63  | 59  | 5  |  | -2 7 -3             | 184 | 166 | 2 |  |
| 7 0 -5              | 379 | 371 | 5  |  | 4 7 -5              | 165 | 166 | 3  |  | -3 4 -4             | 128 | 122 | 2  |  | -1 12 -4            | 149 | 145 | 3  |  | -1 7 -3             | 359 | 352 | 3 |  |
| 9 0 -5              | 85  | 77  | 4  |  | 5 7 -5              | 108 | 111 | 2  |  | -2 4 -4             | 267 | 272 | 3  |  | 0 12 -4             | 43  | 38  | 4  |  | 0 7 -3              | 230 | 224 | 2 |  |
| -3 1 -5             | 292 | 282 | 4  |  | 6 7 -5              | 138 | 138 | 2  |  | -1 4 -4             | 395 | 373 | 6  |  | 1 12 -4             | 159 | 166 | 9  |  | 1 7 -3              | 108 | 114 | 1 |  |
| -2 1 -5             | 89  | 78  | 2  |  | 7 7 -5              | 181 | 179 | 3  |  | 0 4 -4              | 245 | 240 | 1  |  | 2 12 -4             | 41  | 25  | 6  |  | 2 7 -3              | 260 | 253 | 4 |  |
| -1 1 -5             | 186 | 177 | 1  |  | -4 8 -5             | 164 | 173 | 2  |  | 1 4 -4              | 393 | 381 | 3  |  | -1 0 -3             | 574 | 586 | 7  |  | 3 7 -3              | 319 | 308 | 3 |  |
| 0 1 -5              | 409 | 387 | 5  |  | -3 8 -5             | 163 | 160 | 2  |  | 2 4 -4              | 318 | 313 | 5  |  | 3 0 -3              | 558 | 558 | 12 |  | 4 7 -3              | 230 | 230 | 3 |  |
| 1 1 -5              | 266 | 290 | 3  |  | -2 8 -5             | 220 | 211 | 2  |  | 3 4 -4              | 175 | 168 | 5  |  | 5 0 -3              | 495 | 483 | 6  |  | 5 7 -3              | 166 | 165 | 3 |  |
| 2 1 -5              | 234 | 224 | 1  |  | -1 8 -5             | 40  | 30  | 2  |  | 4 4 -4              | 329 | 326 | 6  |  | 7 0 -3              | 53  | 60  | 3  |  | 6 7 -3              | 205 | 208 | 8 |  |
| 3 1 -5              | 310 | 318 | 1  |  | 0 8 -5              | 329 | 334 | 3  |  | 5 4 -4              | 330 | 331 | 5  |  | 9 0 -3              | 255 | 248 | 4  |  | 7 7 -3              | 63  | 53  | 3 |  |
| 4 1 -5              | 201 | 196 | 3  |  | 1 8 -5              | 240 | 238 | 6  |  | 6 4 -4              | 265 | 260 | 3  |  | -2 1 -3             | 106 | 96  | 1  |  | -4 8 -3             | 335 | 335 | 3 |  |
| 5 1 -5              | 122 | 126 | 1  |  | 2 8 -5              | 208 | 210 | 4  |  | 7 4 -4              | 63  | 64  | 2  |  | -1 1 -3             | 436 | 462 | 3  |  | -3 8 -3             | 67  | 63  | 3 |  |
| 6 1 -5              | 171 | 170 | 3  |  | 3 8 -5              | 40  | 32  | 16 |  | 8 4 -4              | 244 | 245 | 5  |  | 0 1 -3              | 517 | 520 | 6  |  | -2 8 -3             | 299 | 297 | 8 |  |
| 7 1 -5              | 280 | 282 | 4  |  | 4 8 -5              | 304 | 308 | 3  |  | 9 4 -4              | 109 | 106 | 3  |  | 1 1 -3              | 491 | 498 | 3  |  | -1 8 -3             | 325 | 318 | 6 |  |
| 8 1 -5              | 79  | 82  | 5  |  | 5 8 -5              | 126 | 125 | 1  |  | -3 5 -4             | 109 | 119 | 2  |  | 2 1 -3              | 302 | 291 | 1  |  | 0 8 -3              | 310 | 316 | 3 |  |
| 9 1 -5              | 114 | 119 | 3  |  | 6 8 -5              | 142 | 145 | 3  |  | -2 5 -4             | 278 | 281 | 3  |  | 3 1 -3              | 435 | 449 | 5  |  | 1 8 -3              | 41  | 45  | 2 |  |
| -3 2 -5             | 354 | 332 | 4  |  | 7 8 -5              | 70  | 75  | 8  |  | -1 5 -4             | 394 | 388 | 3  |  | 4 1 -3              | 199 | 179 | 2  |  | 2 8 -3              | 313 | 312 | 3 |  |
| -2 2 -5             | 212 | 201 | 3  |  | -4 9 -5             | 159 | 160 | 2  |  | 0 5 -4              | 312 | 301 | 2  |  | 5 1 -3              | 417 | 403 | 5  |  | 3 8 -3              | 238 | 238 | 3 |  |
| -1 2 -5             | 652 | 635 | 9  |  | -3 9 -5             | 56  | 53  | 2  |  | 1 5 -4              | 522 | 521 | 3  |  | 6 1 -3              | 203 | 200 | 2  |  | 4 8 -3              | 192 | 191 | 3 |  |
| 0 2 -5              | 130 | 128 | 5  |  | -2 9 -5             | 229 | 219 | 3  |  | 2 5 -4              | 268 | 268 | 5  |  | 7 1 -3              | 154 | 152 | 2  |  | 5 8 -3              | 165 | 171 | 4 |  |
| 1 2 -5              | 285 | 287 | 1  |  | -1 9 -5             | 137 | 129 | 4  |  | 3 5 -4              | 66  | 69  | 1  |  | 8 1 -3              | 82  | 81  | 3  |  | 6 8 -3              | 181 | 178 | 3 |  |
| 2 2 -5              | 70  | 68  | 3  |  | 0 9 -5              | 293 | 295 | 6  |  | 4 5 -4              | 256 | 255 | 5  |  | 9 1 -3              | 224 | 227 | 2  |  | 7 8 -3              | 69  | 72  | 3 |  |
| 3 2 -5              | 490 | 476 | 8  |  | 1 9 -5              | 37  | 21  | 5  |  | 5 5 -4              | 435 | 441 | 7  |  | -3 2 -3             | 467 | 444 | 6  |  | -3 9 -3             | 70  | 57  | 2 |  |
| 4 2 -5              | 134 | 133 | 4  |  | 2 9 -5              | 177 | 173 | 4  |  | 6 5 -4              | 133 | 136 | 3  |  | -2 2 -3             | 80  | 73  | 1  |  | -2 9 -3             | 305 | 317 | 9 |  |
| 5 2 -5              | 303 | 301 | 8  |  | 3 9 -5              | 48  | 59  | 3  |  | 7 5 -4              | 177 | 171 | 2  |  | -1 2 -3             | 110 | 107 | 2  |  | -1 9 -3             | 104 | 100 | 2 |  |
| 6 2 -5              | 172 | 167 | 3  |  | 4 9 -5              | 294 | 295 | 3  |  | 8 5 -4              | 170 | 174 | 3  |  | 0 2 -3              | 83  | 65  | 1  |  | 0 9 -3              | 300 | 295 | 3 |  |
| 7 2 -5              | 155 | 160 | 3  |  | 5 9 -5              | 108 | 114 | 8  |  | -4 6 -4             | 300 | 308 | 3  |  | 1 2 -3              | 669 | 660 | 13 |  | 1 9 -3              | 138 | 138 | 2 |  |
| 8 2 -5              | 55  | 52  | 3  |  | 6 9 -5              | 110 | 110 | 2  |  | -3 6 -4             | 141 | 154 | 2  |  | 2 2 -3              | 284 | 280 | 4  |  | 2 9 -3              | 314 | 318 | 5 |  |
| 9 2 -5              | 157 | 152 | 3  |  | -3 10 -5            | 20  | 20  | 20 |  | -2 6 -4             | 159 | 150 | 3  |  | 3 2 -3              | 257 | 254 | 5  |  | 3 9 -3              | 48  | 33  | 3 |  |
| -3 3 -5             | 245 | 218 | 3  |  | -2 10 -5            | 235 | 229 | 5  |  | -1 6 -4             | 297 | 283 | 2  |  | 4 2 -3              | 53  | 47  | 4  |  | 4 9 -3              | 150 | 155 | 1 |  |
| -2 3 -5             | 181 | 170 | 2  |  | -1 10 -5            | 169 | 171 | 2  |  | 0 6 -4              | 409 | 386 | 3  |  | 5 2 -3              | 293 | 280 | 4  |  | 5 9 -3              | 43  | 40  | 3 |  |
| -1 3 -5             | 556 | 539 | 7  |  | 0 10 -5             | 263 | 262 | 4  |  | 1 6 -4              | 380 | 398 | 3  |  | 6 2 -3              | 210 | 207 | 2  |  | 6 9 -3              | 201 | 189 | 2 |  |
| 0 3 -5              | 153 | 142 | 4  |  | 1 10 -5             | 96  | 96  | 2  |  | 2 6 -4              | 188 | 181 | 2  |  | 7 2 -3              | 301 | 299 | 3  |  | -2 10 -3            | 135 | 141 | 2 |  |
| 1 3 -5              | 208 | 210 | 1  |  | 2 10 -5             | 151 | 156 | 2  |  | 3 6 -4              | 102 | 98  | 3  |  | 8 2 -3              | 40  | 34  | 4  |  | -1 10 -3            | 140 | 141 | 2 |  |
| 2 3 -5              | 253 | 258 | 4  |  | 3 10 -5             | 101 | 105 | 4  |  | 4 6 -4              | 281 | 282 | 5  |  | 9 2 -3              | 113 | 116 | 2  |  | 0 10 -3             | 182 | 177 | 2 |  |
| 3 3 -5              | 404 | 396 | 14 |  | 4 10 -5             | 227 | 234 | 3  |  | 5 6 -4              | 261 | 271 | 6  |  | -3 3 -3             | 568 | 540 | 7  |  | 1 10 -3             | 125 | 120 | 2 |  |
| 4 3 -5              | 275 | 276 | 6  |  | 5 10 -5             | 136 | 137 | 3  |  | 6 6 -4              | 121 | 125 | 4  |  | -2 3 -3             | 162 | 156 | 2  |  | 2 10 -3             | 244 | 240 | 2 |  |
| 5 3 -5              | 371 | 369 | 4  |  | -3 11 -5            | 56  | 60  | 5  |  | 7 6 -4              | 127 | 127 | 8  |  | -1 3 -3             | 488 | 463 | 6  |  | 3 10 -3             | 78  | 78  | 2 |  |
| 6 3 -5              | 253 | 250 | 7  |  | -2 11 -5            | 86  | 94  | 3  |  | 8 6 -4              | 66  | 65  | 7  |  | 0 3 -3              | 563 | 535 | 6  |  | 5 10 -3             | 109 | 106 | 2 |  |
| 7 3 -5              | 93  | 96  | 3  |  | -1 11 -5            | 43  | 44  | 4  |  | -4 7 -4             | 220 | 220 | 2  |  | 1 3 -3              | 821 | 813 | 11 |  | 6 10 -3             | 208 | 201 | 3 |  |
| 8 3 -5              | 151 | 151 | 3  |  | 0 11 -5             | 137 | 136 | 2  |  | -3 7 -4             | 191 | 191 | 1  |  | 2 3 -3              | 382 | 367 | 16 |  | -2 11 -3            | 222 | 214 | 2 |  |
| -4 4 -5             | 243 | 216 | 3  |  | 1 11 -5             | 67  | 63  | 3  |  | -2 7 -4             | 72  | 65  | 1  |  | 3 3 -3              | 281 | 278 | 6  |  | -1 11 -3            | 58  | 59  | 3 |  |
| -3 4 -5             | 300 | 272 | 4  |  | 2 11 -5             | 153 | 158 | 2  |  | -1 7 -4             | 152 | 150 | 2  |  | 4 3 -3              | 203 | 192 | 4  |  | 0 11 -3             | 253 | 247 | 2 |  |
| -2 4 -5             | 191 | 176 | 3  |  | 3 11 -5             | 91  | 100 | 2  |  | 0 7 -4              | 355 | 349 | 3  |  | 5 3 -3              | 396 | 390 | 6  |  | 1 11 -3             | 62  | 58  | 3 |  |
| -1 4 -5             | 522 | 504 | 6  |  | 4 11 -5             | 155 | 162 | 3  |  | 1 7 -4              | 154 | 152 | 3  |  | 6 3 -3              | 200 | 192 | 3  |  | 2 11 -3             | 175 | 173 | 4 |  |
| 0 4 -5              | 274 | 265 | 2  |  | -2 0 -4             | 166 | 170 | 2  |  | 2 7 -4              | 110 | 115 | 2  |  | 7 3 -3              | 323 | 326 | 3  |  | 3 11 -3             | 64  | 69  | 4 |  |
| 1 4 -5              | 342 | 338 | 3  |  | 2 0 -4              | 233 | 258 | 1  |  | 3 7 -4              | 204 | 198 | 3  |  | 8 3 -3              | 76  | 78  | 6  |  | 4 11 -3             | 199 | 194 | 3 |  |
| 2 4 -5              | 279 | 267 | 7  |  | 4 0                 |     |     |    |  |                     |     |     |    |  |                     |     |     |    |  |                     |     |     |   |  |

Table 6. 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 |   |    |   |   |     |     |   |    |    |   |     |      |    |
|---------------------|---|----|-----|---------------------|----|----|----|---------------------|-----|------|----|---------------------|----|----|-----|---------------------|---|----|---|---|-----|-----|---|----|----|---|-----|------|----|
| 1                   | 3 | -2 | 250 | 249                 | 3  | -1 | 11 | -2                  | 207 | 211  | 2  | 8                   | 6  | -1 | 180 | 169                 | 2 | 6  | 3 | 0 | 48  | 46  | 1 | 1  | 13 | 0 | 243 | 238  | 4  |
| 2                   | 3 | -2 | 609 | 611                 | 20 | 0  | 11 | -2                  | 64  | 63   | 4  | -3                  | 7  | -1 | 357 | 352                 | 4 | 7  | 3 | 0 | 184 | 182 | 2 | 1  | 0  | 1 | 234 | 252  | 2  |
| 3                   | 3 | -2 | 57  | 43                  | 2  | 1  | 11 | -2                  | 241 | 227  | 6  | -2                  | 7  | -1 | 472 | 480                 | 4 | 8  | 3 | 0 | 183 | 181 | 3 | 3  | 0  | 1 | 676 | 703  | 6  |
| 4                   | 3 | -2 | 403 | 389                 | 6  | 2  | 11 | -2                  | 83  | 81   | 2  | -1                  | 7  | -1 | 276 | 278                 | 2 | 9  | 3 | 0 | 43  | 64  | 6 | 5  | 0  | 1 | 455 | 458  | 4  |
| 5                   | 3 | -2 | 282 | 278                 | 3  | 3  | 11 | -2                  | 264 | 258  | 4  | 0                   | 7  | -1 | 432 | 444                 | 3 | -3 | 4 | 0 | 287 | 272 | 2 | 7  | 0  | 1 | 239 | 245  | 5  |
| 6                   | 3 | -2 | 398 | 393                 | 9  | 4  | 11 | -2                  | 68  | 62   | 4  | 1                   | 7  | -1 | 360 | 358                 | 2 | -2 | 4 | 0 | 431 | 456 | 3 | 0  | 1  | 1 | 216 | 223  | 2  |
| 7                   | 3 | -2 | 29  | 21                  | 5  | 5  | 11 | -2                  | 95  | 93   | 4  | 2                   | 7  | -1 | 354 | 347                 | 2 | -1 | 4 | 0 | 335 | 350 | 4 | 1  | 1  | 1 | 571 | 556  | 5  |
| 8                   | 3 | -2 | 130 | 126                 | 5  | -1 | 12 | -2                  | 173 | 177  | 2  | 3                   | 7  | -1 | 149 | 149                 | 2 | 0  | 4 | 0 | 116 | 128 | 2 | 2  | 1  | 1 | 998 | 1018 | 6  |
| 9                   | 3 | -2 | 99  | 104                 | 3  | 0  | 12 | -2                  | 38  | 35   | 4  | 4                   | 7  | -1 | 357 | 355                 | 9 | 1  | 4 | 0 | 339 | 334 | 6 | 3  | 1  | 1 | 744 | 731  | 5  |
| -2                  | 4 | -2 | 458 | 445                 | 6  | 1  | 12 | -2                  | 200 | 198  | 10 | 5                   | 7  | -1 | 125 | 123                 | 3 | 2  | 4 | 0 | 424 | 436 | 3 | 4  | 1  | 1 | 294 | 274  | 4  |
| -1                  | 4 | -2 | 247 | 246                 | 2  | 2  | 12 | -2                  | 49  | 54   | 5  | 6                   | 7  | -1 | 175 | 171                 | 2 | 3  | 4 | 0 | 288 | 283 | 5 | 5  | 1  | 1 | 416 | 408  | 3  |
| 0                   | 4 | -2 | 839 | 829                 | 5  | 3  | 12 | -2                  | 302 | 287  | 4  | 7                   | 7  | -1 | 196 | 194                 | 2 | 4  | 4 | 0 | 304 | 305 | 5 | 6  | 1  | 1 | 255 | 250  | 1  |
| 1                   | 4 | -2 | 327 | 320                 | 3  | 0  | 13 | -2                  | 106 | 105  | 4  | 8                   | 7  | -1 | 119 | 115                 | 3 | 5  | 4 | 0 | 244 | 244 | 2 | 7  | 1  | 1 | 251 | 252  | 2  |
| 2                   | 4 | -2 | 656 | 648                 | 16 | -1 | 0  | -1                  | 239 | 216  | 3  | -3                  | 8  | -1 | 163 | 169                 | 2 | 6  | 4 | 0 | 131 | 134 | 1 | 8  | 1  | 1 | 168 | 179  | 3  |
| 3                   | 4 | -2 | 343 | 334                 | 8  | 1  | 0  | -1                  | 892 | 1022 | 44 | -2                  | 8  | -1 | 430 | 400                 | 4 | 7  | 4 | 0 | 158 | 156 | 3 | 9  | 1  | 1 | 227 | 231  | 4  |
| 4                   | 4 | -2 | 538 | 506                 | 6  | 3  | 0  | -1                  | 72  | 52   | 1  | -1                  | 8  | -1 | 204 | 211                 | 6 | 8  | 4 | 0 | 166 | 156 | 2 | -2 | 2  | 1 | 261 | 254  | 2  |
| 5                   | 4 | -2 | 97  | 97                  | 1  | 5  | 0  | -1                  | 435 | 426  | 4  | 0                   | 8  | -1 | 169 | 170                 | 1 | -3 | 5 | 0 | 181 | 176 | 1 | -1 | 2  | 1 | 287 | 317  | 3  |
| 6                   | 4 | -2 | 326 | 317                 | 2  | 7  | 0  | -1                  | 278 | 273  | 4  | 1                   | 8  | -1 | 233 | 241                 | 2 | -2 | 5 | 0 | 468 | 453 | 6 | 0  | 2  | 1 | 632 | 647  | 5  |
| 7                   | 4 | -2 | 156 | 162                 | 4  | 9  | 0  | -1                  | 59  | 57   | 4  | 2                   | 8  | -1 | 163 | 151                 | 3 | -1 | 5 | 0 | 362 | 364 | 3 | 1  | 2  | 1 | 295 | 319  | 4  |
| 8                   | 4 | -2 | 142 | 143                 | 3  | -1 | 1  | -1                  | 568 | 557  | 7  | 3                   | 8  | -1 | 201 | 200                 | 1 | 0  | 5 | 0 | 274 | 268 | 3 | 2  | 2  | 1 | 303 | 304  | 2  |
| -3                  | 5 | -2 | 274 | 267                 | 2  | 0  | 1  | -1                  | 216 | 215  | 1  | 4                   | 8  | -1 | 182 | 176                 | 4 | 1  | 5 | 0 | 360 | 350 | 2 | 3  | 2  | 1 | 246 | 251  | 2  |
| -2                  | 5 | -2 | 95  | 88                  | 1  | 1  | 1  | -1                  | 927 | 960  | 48 | 5                   | 8  | -1 | 128 | 134                 | 3 | 2  | 5 | 0 | 465 | 455 | 7 | 4  | 2  | 1 | 282 | 273  | 3  |
| -1                  | 5 | -2 | 162 | 172                 | 1  | 2  | 1  | -1                  | 695 | 693  | 6  | 6                   | 8  | -1 | 133 | 132                 | 2 | 3  | 5 | 0 | 177 | 183 | 4 | 5  | 2  | 1 | 243 | 238  | 2  |
| 0                   | 5 | -2 | 112 | 110                 | 3  | 3  | 1  | -1                  | 240 | 239  | 3  | 7                   | 8  | -1 | 150 | 147                 | 2 | 4  | 5 | 0 | 234 | 228 | 5 | 6  | 2  | 1 | 114 | 114  | 1  |
| 1                   | 5 | -2 | 62  | 71                  | 1  | 4  | 1  | -1                  | 106 | 106  | 1  | -2                  | 9  | -1 | 365 | 361                 | 5 | 5  | 5 | 0 | 333 | 323 | 5 | 7  | 2  | 1 | 208 | 211  | 2  |
| 2                   | 5 | -2 | 90  | 102                 | 1  | 5  | 1  | -1                  | 472 | 462  | 8  | -1                  | 9  | -1 | 198 | 203                 | 2 | 6  | 5 | 0 | 228 | 225 | 4 | 9  | 2  | 1 | 98  | 100  | 3  |
| 3                   | 5 | -2 | 361 | 359                 | 5  | 6  | 1  | -1                  | 94  | 100  | 1  | 0                   | 9  | -1 | 204 | 209                 | 2 | 7  | 5 | 0 | 117 | 117 | 2 | -3 | 3  | 1 | 571 | 581  | 5  |
| 4                   | 5 | -2 | 134 | 144                 | 2  | 7  | 1  | -1                  | 254 | 247  | 2  | 1                   | 9  | -1 | 71  | 74                  | 1 | 8  | 5 | 0 | 155 | 155 | 4 | -2 | 3  | 1 | 347 | 364  | 4  |
| 5                   | 5 | -2 | 123 | 116                 | 1  | 8  | 1  | -1                  | 68  | 68   | 6  | 2                   | 9  | -1 | 196 | 192                 | 1 | -3 | 6 | 0 | 246 | 241 | 3 | -1 | 3  | 1 | 501 | 534  | 6  |
| 6                   | 5 | -2 | 172 | 169                 | 3  | 9  | 1  | -1                  | 112 | 114  | 3  | 3                   | 9  | -1 | 178 | 180                 | 2 | -2 | 6 | 0 | 374 | 370 | 4 | 0  | 3  | 1 | 288 | 296  | 2  |
| 7                   | 5 | -2 | 178 | 168                 | 1  | -1 | 2  | -1                  | 300 | 316  | 3  | 4                   | 9  | -1 | 241 | 240                 | 3 | -1 | 6 | 0 | 278 | 282 | 3 | 1  | 3  | 1 | 504 | 524  | 9  |
| 8                   | 5 | -2 | 88  | 87                  | 3  | 0  | 2  | -1                  | 632 | 659  | 5  | 5                   | 9  | -1 | 88  | 91                  | 6 | 0  | 6 | 0 | 367 | 377 | 2 | 2  | 3  | 1 | 383 | 388  | 5  |
| -4                  | 6 | -2 | 269 | 254                 | 2  | 1  | 2  | -1                  | 311 | 321  | 5  | 6                   | 9  | -1 | 149 | 156                 | 2 | 1  | 6 | 0 | 283 | 284 | 2 | 3  | 3  | 1 | 295 | 285  | 4  |
| -3                  | 6 | -2 | 286 | 292                 | 2  | 2  | 2  | -1                  | 265 | 243  | 5  | -2                  | 10 | -1 | 208 | 211                 | 3 | 2  | 6 | 0 | 374 | 379 | 2 | 4  | 3  | 1 | 35  | 30   | 2  |
| -2                  | 6 | -2 | 376 | 375                 | 5  | 3  | 2  | -1                  | 413 | 415  | 5  | -1                  | 10 | -1 | 146 | 144                 | 2 | 3  | 6 | 0 | 243 | 243 | 2 | 5  | 3  | 1 | 244 | 241  | 2  |
| -1                  | 6 | -2 | 398 | 408                 | 3  | 4  | 2  | -1                  | 411 | 396  | 8  | 0                   | 10 | -1 | 212 | 212                 | 2 | 4  | 6 | 0 | 265 | 261 | 2 | 6  | 3  | 1 | 157 | 157  | 2  |
| 0                   | 6 | -2 | 95  | 96                  | 1  | 5  | 2  | -1                  | 404 | 392  | 5  | 1                   | 10 | -1 | 139 | 142                 | 8 | 5  | 6 | 0 | 237 | 227 | 5 | 7  | 3  | 1 | 161 | 159  | 2  |
| 1                   | 6 | -2 | 289 | 282                 | 2  | 6  | 2  | -1                  | 57  | 50   | 6  | 2                   | 10 | -1 | 271 | 271                 | 5 | 6  | 6 | 0 | 306 | 298 | 4 | 8  | 3  | 1 | 66  | 62   | 2  |
| 2                   | 6 | -2 | 218 | 206                 | 2  | 7  | 2  | -1                  | 178 | 175  | 3  | 3                   | 10 | -1 | 182 | 175                 | 2 | 7  | 6 | 0 | 158 | 154 | 3 | 9  | 3  | 1 | 16  | 13   | 15 |
| 3                   | 6 | -2 | 347 | 349                 | 4  | 8  | 2  | -1                  | 112 | 107  | 4  | 4                   | 10 | -1 | 283 | 281                 | 6 | 8  | 6 | 0 | 93  | 96  | 2 | -3 | 4  | 1 | 338 | 363  | 4  |
| 4                   | 6 | -2 | 142 | 143                 | 1  | 9  | 2  | -1                  | 233 | 239  | 3  | 5                   | 10 | -1 | 51  | 49                  | 6 | -2 | 7 | 0 | 187 | 185 | 2 | -2 | 4  | 1 | 314 | 340  | 4  |
| 5                   | 6 | -2 | 132 | 136                 | 2  | -2 | 3  | -1                  | 390 | 380  | 5  | 6                   | 10 | -1 | 183 | 189                 | 3 | -1 | 7 | 0 | 295 | 293 | 2 | -1 | 4  | 1 | 162 | 166  | 2  |
| 6                   | 6 | -2 | 29  | 26                  | 8  | -1 | 3  | -1                  | 518 | 543  | 7  | -1                  | 11 | -1 | 67  | 63                  | 2 | 0  | 7 | 0 | 376 | 379 | 2 | 0  | 4  | 1 | 154 | 156  | 2  |
| 7                   | 6 | -2 | 205 | 195                 | 2  | 0  | 3  | -1                  | 293 | 290  | 2  | 0                   | 11 | -1 | 256 | 247                 | 2 | 1  | 7 | 0 | 297 | 296 | 2 | 1  | 4  | 1 | 212 | 233  | 2  |
| 8                   | 6 | -2 | 101 | 87                  | 2  | 1  | 3  | -1                  | 546 | 542  | 8  | 1                   | 11 | -1 | 38  | 41                  | 6 | 2  | 7 | 0 | 190 | 194 | 1 | 2  | 4  | 1 | 66  | 61   | 1  |
| -4                  | 7 | -2 | 97  | 84                  | 2  | 2  | 3  | -1                  | 365 | 345  | 13 | 2                   | 11 | -1 | 325 | 322                 | 4 | 3  | 7 | 0 | 326 | 330 | 3 | 3  | 4  | 1 | 250 | 251  | 1  |
| -3                  | 7 | -2 | 225 | 205                 | 2  | 3  | 3  | -1                  | 579 | 581  | 8  | 3                   | 11 | -1 | 147 | 147                 | 3 | 4  | 7 | 0 | 170 | 166 | 2 | 4  | 4  | 1 | 253 | 256  | 2  |
| -2                  | 7 | -2 | 331 | 331                 | 3  | 4  | 3  | -1                  | 296 | 288  | 3  | 4                   | 11 | -1 | 147 | 139                 | 7 | 5  | 7 | 0 | 149 |     |   |    |    |   |     |      |    |

Table 6. 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 |     |    |    |   |   |     |     |    |    |   |   |     |     |   |
|---------------------|----|-----|-----|-----|---------------------|----|----|---|-----|---------------------|---|----|---|---|---------------------|-----|----|----|---|---|-----|-----|----|----|---|---|-----|-----|---|
| 2                   | 8  | 1   | 420 | 426 | 5                   | 8  | 5  | 2 | 122 | 128                 | 4 | -1 | 4 | 3 | 454                 | 471 | 5  | 8  | 2 | 4 | 188 | 186 | 3  | 3  | 2 | 5 | 319 | 322 | 5 |
| 3                   | 8  | 1   | 155 | 151 | 2                   | -2 | 6  | 2 | 201 | 230                 | 2 | 0  | 4 | 3 | 389                 | 387 | 5  | -2 | 3 | 4 | 386 | 419 | 4  | 4  | 2 | 5 | 58  | 62  | 3 |
| 4                   | 8  | 1   | 144 | 145 | 2                   | -1 | 6  | 2 | 271 | 288                 | 3 | 1  | 4 | 3 | 324                 | 322 | 4  | -1 | 3 | 4 | 255 | 241 | 3  | 5  | 2 | 5 | 259 | 268 | 3 |
| 5                   | 8  | 1   | 60  | 61  | 9                   | 0  | 6  | 2 | 101 | 107                 | 1 | 2  | 4 | 3 | 354                 | 346 | 3  | 0  | 3 | 4 | 167 | 175 | 2  | 6  | 2 | 5 | 180 | 188 | 3 |
| 6                   | 8  | 1   | 299 | 298 | 3                   | 1  | 6  | 2 | 395 | 390                 | 3 | 3  | 4 | 3 | 342                 | 337 | 5  | 1  | 3 | 4 | 134 | 138 | 2  | 7  | 2 | 5 | 247 | 253 | 2 |
| 7                   | 8  | 1   | 67  | 58  | 3                   | 2  | 6  | 2 | 366 | 372                 | 8 | 4  | 4 | 3 | 171                 | 169 | 2  | 2  | 3 | 4 | 430 | 444 | 7  | 8  | 2 | 5 | 47  | 39  | 5 |
| -1                  | 9  | 1   | 72  | 65  | 2                   | 3  | 6  | 2 | 282 | 284                 | 5 | 5  | 4 | 3 | 307                 | 310 | 3  | 3  | 3 | 4 | 266 | 268 | 5  | -2 | 3 | 5 | 239 | 246 | 3 |
| 0                   | 9  | 1   | 204 | 204 | 3                   | 4  | 6  | 2 | 271 | 273                 | 2 | 6  | 4 | 3 | 262                 | 265 | 3  | 4  | 3 | 4 | 206 | 214 | 3  | -1 | 3 | 5 | 194 | 181 | 2 |
| 1                   | 9  | 1   | 197 | 195 | 2                   | 5  | 6  | 2 | 187 | 183                 | 2 | 7  | 4 | 3 | 161                 | 163 | 3  | 5  | 3 | 4 | 29  | 35  | 2  | 0  | 3 | 5 | 149 | 148 | 3 |
| 2                   | 9  | 1   | 375 | 382 | 4                   | 6  | 6  | 2 | 228 | 226                 | 3 | 8  | 4 | 3 | 65                  | 65  | 3  | 6  | 3 | 4 | 184 | 182 | 1  | 1  | 3 | 5 | 535 | 529 | 4 |
| 3                   | 9  | 1   | 79  | 75  | 5                   | 7  | 6  | 2 | 172 | 172                 | 3 | -2 | 5 | 3 | 125                 | 133 | 2  | 7  | 3 | 4 | 114 | 118 | 7  | 2  | 3 | 5 | 173 | 170 | 1 |
| 4                   | 9  | 1   | 96  | 105 | 2                   | 8  | 6  | 2 | 173 | 170                 | 3 | -1 | 5 | 3 | 273                 | 262 | 3  | 8  | 3 | 4 | 210 | 215 | 3  | 3  | 3 | 5 | 232 | 238 | 2 |
| 5                   | 9  | 1   | 110 | 112 | 2                   | -1 | 7  | 2 | 232 | 252                 | 3 | 0  | 5 | 3 | 362                 | 355 | 4  | -2 | 4 | 4 | 314 | 321 | 4  | 4  | 3 | 5 | 64  | 64  | 2 |
| 6                   | 9  | 1   | 234 | 235 | 5                   | 0  | 7  | 2 | 146 | 141                 | 2 | 1  | 5 | 3 | 323                 | 303 | 3  | -1 | 4 | 4 | 379 | 372 | 4  | 5  | 3 | 5 | 213 | 210 | 4 |
| 0                   | 10 | 1   | 215 | 219 | 3                   | 1  | 7  | 2 | 343 | 349                 | 3 | 2  | 5 | 3 | 417                 | 413 | 12 | 0  | 4 | 4 | 238 | 223 | 3  | 6  | 3 | 5 | 170 | 178 | 4 |
| 1                   | 10 | 1   | 140 | 147 | 3                   | 2  | 7  | 2 | 328 | 320                 | 3 | 3  | 5 | 3 | 258                 | 248 | 3  | 1  | 4 | 4 | 393 | 390 | 7  | 7  | 3 | 5 | 210 | 212 | 2 |
| 2                   | 10 | 1   | 212 | 208 | 2                   | 3  | 7  | 2 | 225 | 228                 | 3 | 4  | 5 | 3 | 150                 | 146 | 5  | 2  | 4 | 4 | 266 | 257 | 8  | -1 | 4 | 5 | 319 | 326 | 4 |
| 3                   | 10 | 1   | 168 | 169 | 2                   | 4  | 7  | 2 | 99  | 106                 | 2 | 5  | 5 | 3 | 259                 | 255 | 2  | 3  | 4 | 4 | 117 | 116 | 2  | 0  | 4 | 5 | 264 | 284 | 3 |
| 4                   | 10 | 1   | 76  | 83  | 2                   | 5  | 7  | 2 | 276 | 265                 | 4 | 6  | 5 | 3 | 303                 | 310 | 3  | 4  | 4 | 4 | 193 | 199 | 2  | 1  | 4 | 5 | 493 | 495 | 5 |
| 5                   | 10 | 1   | 27  | 10  | 26                  | 6  | 7  | 2 | 125 | 123                 | 6 | 7  | 5 | 3 | 121                 | 127 | 3  | 5  | 4 | 4 | 239 | 243 | 3  | 2  | 4 | 5 | 181 | 183 | 1 |
| 0                   | 11 | 1   | 260 | 262 | 4                   | 7  | 7  | 2 | 172 | 169                 | 2 | 8  | 5 | 3 | 36                  | 23  | 5  | 6  | 4 | 4 | 154 | 152 | 1  | 3  | 4 | 5 | 288 | 290 | 2 |
| 1                   | 11 | 1   | 66  | 63  | 2                   | -1 | 8  | 2 | 210 | 213                 | 3 | -1 | 6 | 3 | 54                  | 39  | 2  | 7  | 4 | 4 | 89  | 91  | 5  | 4  | 4 | 5 | 217 | 225 | 3 |
| 2                   | 11 | 1   | 241 | 234 | 2                   | 0  | 8  | 2 | 115 | 110                 | 2 | 0  | 6 | 3 | 340                 | 330 | 4  | 8  | 4 | 4 | 192 | 196 | 6  | 5  | 4 | 5 | 214 | 216 | 4 |
| 3                   | 11 | 1   | 135 | 137 | 2                   | 1  | 8  | 2 | 369 | 379                 | 6 | 1  | 6 | 3 | 261                 | 266 | 5  | -1 | 5 | 4 | 512 | 506 | 6  | 6  | 4 | 5 | 67  | 74  | 3 |
| 4                   | 11 | 1   | 243 | 246 | 2                   | 2  | 8  | 2 | 209 | 209                 | 2 | 2  | 6 | 3 | 238                 | 253 | 7  | 0  | 5 | 4 | 309 | 306 | 4  | 7  | 4 | 5 | 182 | 187 | 7 |
| 1                   | 12 | 1   | 95  | 87  | 3                   | 3  | 8  | 2 | 123 | 127                 | 2 | 3  | 6 | 3 | 156                 | 155 | 5  | 1  | 5 | 4 | 399 | 400 | 8  | -1 | 5 | 5 | 257 | 259 | 3 |
| 2                   | 12 | 1   | 123 | 113 | 2                   | 4  | 8  | 2 | 35  | 26                  | 3 | 4  | 6 | 3 | 67                  | 57  | 6  | 2  | 5 | 4 | 280 | 277 | 2  | 0  | 5 | 5 | 243 | 254 | 3 |
| 3                   | 12 | 1   | 127 | 128 | 9                   | 5  | 8  | 2 | 252 | 249                 | 3 | 5  | 6 | 3 | 136                 | 138 | 1  | 3  | 5 | 4 | 101 | 97  | 1  | 1  | 5 | 5 | 291 | 288 | 4 |
| 1                   | 13 | 1   | 84  | 82  | 4                   | 6  | 8  | 2 | 85  | 86                  | 4 | 6  | 6 | 3 | 152                 | 148 | 2  | 4  | 5 | 4 | 252 | 247 | 2  | 2  | 5 | 5 | 187 | 187 | 3 |
| 0                   | 0  | 2   | 320 | 304 | 4                   | -1 | 9  | 2 | 302 | 291                 | 4 | 7  | 6 | 3 | 84                  | 88  | 2  | 5  | 5 | 4 | 312 | 316 | 5  | 3  | 5 | 5 | 202 | 206 | 3 |
| 2                   | 0  | 2   | 341 | 364 | 3                   | 0  | 9  | 2 | 216 | 216                 | 3 | -1 | 7 | 3 | 100                 | 110 | 2  | 6  | 5 | 4 | 141 | 140 | 1  | 4  | 5 | 5 | 301 | 304 | 4 |
| 4                   | 0  | 2   | 240 | 251 | 2                   | 1  | 9  | 2 | 329 | 336                 | 3 | 0  | 7 | 3 | 226                 | 222 | 3  | 7  | 5 | 4 | 86  | 85  | 7  | 5  | 5 | 5 | 160 | 165 | 2 |
| 6                   | 0  | 2   | 63  | 61  | 4                   | 2  | 9  | 2 | 98  | 103                 | 2 | 1  | 7 | 3 | 350                 | 347 | 3  | -1 | 6 | 4 | 380 | 377 | 5  | 6  | 5 | 5 | 29  | 7   | 6 |
| -1                  | 1  | 2   | 274 | 291 | 3                   | 3  | 9  | 2 | 159 | 156                 | 2 | 2  | 7 | 3 | 178                 | 183 | 2  | 0  | 6 | 4 | 400 | 395 | 5  | 7  | 5 | 5 | 122 | 125 | 2 |
| 0                   | 1  | 2   | 234 | 222 | 2                   | 4  | 9  | 2 | 121 | 117                 | 3 | 3  | 7 | 3 | 103                 | 110 | 3  | 1  | 6 | 4 | 294 | 300 | 3  | 0  | 6 | 5 | 183 | 194 | 2 |
| 1                   | 1  | 2   | 398 | 392 | 3                   | 5  | 9  | 2 | 243 | 249                 | 2 | 4  | 7 | 3 | 227                 | 230 | 3  | 2  | 6 | 4 | 164 | 155 | 4  | 1  | 6 | 5 | 99  | 111 | 3 |
| 2                   | 1  | 2   | 427 | 452 | 2                   | 6  | 9  | 2 | 138 | 141                 | 2 | 5  | 7 | 3 | 89                  | 88  | 3  | 3  | 6 | 4 | 134 | 134 | 2  | 2  | 6 | 5 | 216 | 210 | 4 |
| 3                   | 1  | 2   | 182 | 178 | 1                   | 0  | 10 | 2 | 191 | 198                 | 3 | 6  | 7 | 3 | 144                 | 146 | 2  | 4  | 6 | 4 | 298 | 302 | 4  | 3  | 6 | 5 | 174 | 178 | 3 |
| 4                   | 1  | 2   | 331 | 335 | 2                   | 1  | 10 | 2 | 273 | 271                 | 2 | 7  | 7 | 3 | 71                  | 73  | 3  | 5  | 6 | 4 | 218 | 223 | 4  | 4  | 6 | 5 | 204 | 208 | 7 |
| 5                   | 1  | 2   | 136 | 135 | 1                   | 2  | 10 | 2 | 117 | 121                 | 4 | 0  | 8 | 3 | 296                 | 334 | 4  | 6  | 6 | 4 | 142 | 143 | 2  | 5  | 6 | 5 | 197 | 201 | 2 |
| 6                   | 1  | 2   | 137 | 137 | 2                   | 3  | 10 | 2 | 158 | 154                 | 2 | 1  | 8 | 3 | 306                 | 318 | 3  | 7  | 6 | 4 | 110 | 111 | 8  | 6  | 6 | 5 | 63  | 61  | 3 |
| 7                   | 1  | 2   | 160 | 168 | 1                   | 4  | 10 | 2 | 119 | 121                 | 6 | 2  | 8 | 3 | 286                 | 282 | 3  | 0  | 7 | 4 | 349 | 352 | 4  | 7  | 6 | 5 | 57  | 61  | 5 |
| 8                   | 1  | 2   | 249 | 255 | 4                   | 5  | 10 | 2 | 242 | 245                 | 4 | 3  | 8 | 3 | 78                  | 72  | 2  | 1  | 7 | 4 | 150 | 157 | 2  | 0  | 7 | 5 | 183 | 174 | 3 |
| -1                  | 2  | 2   | 306 | 290 | 3                   | 1  | 11 | 2 | 209 | 206                 | 3 | 4  | 8 | 3 | 336                 | 340 | 9  | 2  | 7 | 4 | 69  | 73  | 10 | 1  | 7 | 5 | 124 | 134 | 2 |
| 0                   | 2  | 2   | 785 | 784 | 16                  | 2  | 11 | 2 | 118 | 113                 | 3 | 5  | 8 | 3 | 157                 | 154 | 3  | 3  | 7 | 4 | 184 | 182 | 2  | 2  | 7 | 5 | 126 | 126 | 3 |
| 1                   | 2  | 2   | 377 | 379 | 4                   | 3  | 11 | 2 | 212 | 217                 | 2 | 6  | 8 | 3 | 107                 | 113 | 2  | 4  | 7 | 4 | 212 | 218 | 3  | 3  | 7 | 5 | 167 | 167 | 2 |
| 2                   | 2  | 2   | 368 | 359 | 4                   | 4  | 11 | 2 | 80  | 81                  | 3 | 0  | 9 | 3 | 287                 | 309 | 4  | 5  | 7 | 4 | 91  | 97  | 3  | 4  | 7 | 5 | 137 | 143 | 3 |
| 3                   | 2  | 2   | 203 | 201 | 2                   | 1  | 12 | 2 | 171 | 169                 | 3 | 1  | 9 | 3 | 101                 | 108 | 2  | 6  | 7 | 4 | 165 | 172 | 5  | 5  | 7 | 5 | 120 | 127 | 2 |
| 4                   | 2  | 2</ |     |     |                     |    |    |   |     |                     |   |    |   |   |                     |     |    |    |   |   |     |     |    |    |   |   |     |     |   |

Table 6. Observed and calculated structure factors for 1

Page 5

| 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 | 3 | 6 | 238  | 243  | 3   | 3  | 9  | 6 | 110  | 106  | 2   | 2  | 5 | 7 | 213  | 208  | 9   | 4  | 3 | 8 | 125  | 128  | 3   | 1  | 4 | 9  | 239  | 244  | 11  |
| 0  | 3 | 6 | 483  | 493  | 8   | 4  | 9  | 6 | 93   | 97   | 3   | 3  | 5 | 7 | 160  | 163  | 5   | 5  | 3 | 8 | 27   | 8    | 13  | 2  | 4 | 9  | 103  | 99   | 5   |
| 1  | 3 | 6 | 156  | 157  | 1   | 2  | 10 | 6 | 49   | 71   | 5   | 4  | 5 | 7 | 63   | 66   | 2   | 0  | 4 | 8 | 163  | 170  | 2   | 3  | 4 | 9  | 141  | 148  | 2   |
| 2  | 3 | 6 | 333  | 334  | 4   | 3  | 10 | 6 | 114  | 124  | 3   | 5  | 5 | 7 | 94   | 90   | 5   | 1  | 4 | 8 | 218  | 223  | 9   | 4  | 4 | 9  | 152  | 149  | 5   |
| 3  | 3 | 6 | 110  | 112  | 3   | -1 | 0  | 7 | 267  | 253  | 3   | 6  | 5 | 7 | 142  | 146  | 13  | 2  | 4 | 8 | 249  | 250  | 10  | 1  | 5 | 9  | 146  | 159  | 3   |
| 4  | 3 | 6 | 328  | 334  | 6   | 1  | 0  | 7 | 671  | 682  | 8   | 1  | 6 | 7 | 344  | 350  | 4   | 3  | 4 | 8 | 114  | 108  | 2   | 2  | 5 | 9  | 80   | 71   | 6   |
| 5  | 3 | 6 | 194  | 200  | 4   | 3  | 0  | 7 | 90   | 91   | 2   | 2  | 6 | 7 | 350  | 360  | 4   | 4  | 4 | 8 | 171  | 175  | 2   | 3  | 5 | 9  | 127  | 124  | 2   |
| 6  | 3 | 6 | 247  | 252  | 3   | 5  | 0  | 7 | 289  | 294  | 4   | 3  | 6 | 7 | 226  | 229  | 5   | 5  | 4 | 8 | 178  | 176  | 2   | 4  | 5 | 9  | 187  | 187  | 3   |
| 7  | 3 | 6 | 69   | 62   | 4   | -2 | 1  | 7 | 167  | 158  | 2   | 4  | 6 | 7 | 214  | 223  | 6   | 1  | 5 | 8 | 165  | 169  | 3   | 2  | 6 | 9  | 140  | 148  | 3   |
| -1 | 4 | 6 | 80   | 89   | 2   | -1 | 1  | 7 | 278  | 264  | 2   | 5  | 6 | 7 | 233  | 234  | 4   | 2  | 5 | 8 | 205  | 210  | 6   | 3  | 6 | 9  | 164  | 167  | 3   |
| 0  | 4 | 6 | 156  | 150  | 2   | 0  | 1  | 7 | 191  | 196  | 2   | 1  | 7 | 7 | 210  | 229  | 3   | 3  | 5 | 8 | 109  | 105  | 2   | 3  | 7 | 9  | 137  | 130  | 3   |
| 1  | 4 | 6 | 26   | 5    | 5   | 1  | 1  | 7 | 522  | 529  | 4   | 2  | 7 | 7 | 147  | 162  | 3   | 4  | 5 | 8 | 123  | 126  | 2   | 0  | 0 | 10 | 76   | 81   | 3   |
| 2  | 4 | 6 | 141  | 147  | 1   | 2  | 1  | 7 | 148  | 148  | 2   | 3  | 7 | 7 | 167  | 173  | 2   | 5  | 5 | 8 | 220  | 217  | 4   | 2  | 0 | 10 | 266  | 258  | 4   |
| 3  | 4 | 6 | 142  | 141  | 3   | 3  | 1  | 7 | 165  | 168  | 2   | 4  | 7 | 7 | 166  | 164  | 3   | 1  | 6 | 8 | 151  | 162  | 3   | -1 | 1 | 10 | 160  | 161  | 3   |
| 4  | 4 | 6 | 213  | 215  | 6   | 4  | 1  | 7 | 79   | 83   | 3   | 5  | 7 | 7 | 74   | 83   | 4   | 2  | 6 | 8 | 152  | 168  | 3   | 0  | 1 | 10 | 125  | 124  | 2   |
| 5  | 4 | 6 | 98   | 101  | 5   | 5  | 1  | 7 | 289  | 290  | 3   | 2  | 8 | 7 | 150  | 153  | 3   | 3  | 6 | 8 | 111  | 119  | 3   | 1  | 1 | 10 | 62   | 70   | 3   |
| 6  | 4 | 6 | 220  | 228  | 6   | 6  | 1  | 7 | 25   | 11   | 12  | 3  | 8 | 7 | 96   | 111  | 2   | 4  | 6 | 8 | 134  | 137  | 6   | 2  | 1 | 10 | 177  | 177  | 2   |
| 7  | 4 | 6 | 92   | 87   | 3   | -1 | 2  | 7 | 382  | 383  | 8   | 4  | 8 | 7 | 166  | 181  | 3   | 2  | 7 | 8 | 99   | 115  | 3   | 3  | 1 | 10 | 76   | 81   | 2   |
| 0  | 5 | 6 | 431  | 438  | 5   | 0  | 2  | 7 | 136  | 144  | 3   | 2  | 9 | 7 | 123  | 128  | 3   | 3  | 7 | 8 | 217  | 236  | 3   | 0  | 2 | 10 | 244  | 241  | 5   |
| 1  | 5 | 6 | 188  | 200  | 3   | 1  | 2  | 7 | 331  | 343  | 6   | 3  | 9 | 7 | 102  | 100  | 3   | 4  | 7 | 8 | 174  | 181  | 8   | 1  | 2 | 10 | 91   | 93   | 5   |
| 2  | 5 | 6 | 268  | 265  | 7   | 2  | 2  | 7 | 220  | 220  | 2   | -2 | 0 | 8 | 213  | 192  | 3   | 2  | 8 | 8 | 54   | 56   | 4   | 2  | 2 | 10 | 107  | 104  | 3   |
| 3  | 5 | 6 | 374  | 376  | 6   | 3  | 2  | 7 | 301  | 303  | 2   | 0  | 0 | 8 | 530  | 525  | 6   | 3  | 8 | 8 | 186  | 202  | 3   | 3  | 2 | 10 | 75   | 56   | 3   |
| 4  | 5 | 6 | 266  | 270  | 3   | 4  | 2  | 7 | 115  | 113  | 2   | 2  | 0 | 8 | 141  | 140  | 3   | -1 | 0 | 9 | 324  | 339  | 4   | 0  | 3 | 10 | 375  | 368  | 5   |
| 5  | 5 | 6 | 80   | 89   | 3   | 5  | 2  | 7 | 265  | 270  | 2   | 4  | 0 | 8 | 337  | 334  | 4   | 1  | 0 | 9 | 92   | 99   | 3   | 1  | 3 | 10 | 103  | 105  | 5   |
| 6  | 5 | 6 | 140  | 139  | 2   | 6  | 2  | 7 | 81   | 84   | 3   | -1 | 1 | 8 | 150  | 157  | 2   | 3  | 0 | 9 | 343  | 343  | 5   | 2  | 3 | 10 | 159  | 166  | 2   |
| 0  | 6 | 6 | 125  | 112  | 2   | -1 | 3  | 7 | 143  | 139  | 2   | 0  | 1 | 8 | 551  | 569  | 5   | -1 | 1 | 9 | 240  | 236  | 5   | 3  | 3 | 10 | 53   | 68   | 7   |
| 1  | 6 | 6 | 144  | 139  | 2   | 0  | 3  | 7 | 218  | 233  | 6   | 1  | 1 | 8 | 181  | 182  | 3   | 0  | 1 | 9 | 173  | 176  | 2   | 1  | 4 | 10 | 129  | 126  | 7   |
| 2  | 6 | 6 | 80   | 79   | 3   | 1  | 3  | 7 | 78   | 72   | 2   | 2  | 1 | 8 | 295  | 296  | 3   | 1  | 1 | 9 | 82   | 72   | 2   | 2  | 4 | 10 | 129  | 125  | 8   |
| 3  | 6 | 6 | 259  | 269  | 2   | 2  | 3  | 7 | 76   | 79   | 2   | 3  | 1 | 8 | 77   | 80   | 2   | 2  | 1 | 9 | 110  | 114  | 7   | 3  | 4 | 10 | 103  | 101  | 3   |
| 4  | 6 | 6 | 76   | 73   | 5   | 3  | 3  | 7 | 138  | 137  | 3   | 4  | 1 | 8 | 366  | 369  | 3   | 3  | 1 | 9 | 162  | 161  | 4   | 2  | 5 | 10 | 90   | 104  | 3   |
| 5  | 6 | 6 | 113  | 118  | 2   | 4  | 3  | 7 | 182  | 196  | 3   | 5  | 1 | 8 | 115  | 113  | 2   | 4  | 1 | 9 | 64   | 64   | 12  | 1  | 0 | 11 | 296  | 295  | 4   |
| 6  | 6 | 6 | 51   | 38   | 7   | 5  | 3  | 7 | 194  | 200  | 2   | -1 | 2 | 8 | 292  | 296  | 9   | -1 | 2 | 9 | 264  | 275  | 4   | 0  | 1 | 11 | 146  | 140  | 3   |
| 1  | 7 | 6 | 208  | 212  | 3   | 6  | 3  | 7 | 64   | 60   | 3   | 0  | 2 | 8 | 75   | 64   | 1   | 0  | 2 | 9 | 93   | 93   | 2   | 1  | 1 | 11 | 164  | 167  | 3   |
| 2  | 7 | 6 | 167  | 177  | 2   | 0  | 4  | 7 | 121  | 113  | 2   | 1  | 2 | 8 | 41   | 38   | 2   | 1  | 2 | 9 | 298  | 298  | 4   | 2  | 1 | 11 | 43   | 41   | 16  |
| 3  | 7 | 6 | 163  | 164  | 2   | 1  | 4  | 7 | 88   | 89   | 1   | 2  | 2 | 8 | 87   | 80   | 2   | 2  | 2 | 9 | 206  | 215  | 2   | 0  | 2 | 11 | 118  | 123  | 3   |
| 4  | 7 | 6 | 159  | 162  | 4   | 2  | 4  | 7 | 214  | 215  | 2   | 3  | 2 | 8 | 266  | 274  | 2   | 3  | 2 | 9 | 161  | 157  | 7   | 1  | 2 | 11 | 58   | 50   | 5   |
| 5  | 7 | 6 | 142  | 150  | 2   | 3  | 4  | 7 | 262  | 259  | 6   | 4  | 2 | 8 | 62   | 69   | 2   | 4  | 2 | 9 | 65   | 74   | 8   | 2  | 2 | 11 | 35   | 46   | 8   |
| 1  | 8 | 6 | 213  | 222  | 3   | 4  | 4  | 7 | 31   | 14   | 4   | 5  | 2 | 8 | 83   | 83   | 2   | 0  | 3 | 9 | 152  | 160  | 6   | 1  | 3 | 11 | 123  | 121  | 3   |
| 2  | 8 | 6 | 128  | 144  | 3   | 5  | 4  | 7 | 155  | 166  | 3   | 0  | 3 | 8 | 67   | 69   | 2   | 1  | 3 | 9 | 308  | 317  | 6   | 2  | 3 | 11 | 55   | 45   | 5   |
| 3  | 8 | 6 | 176  | 176  | 2   | 6  | 4  | 7 | 122  | 115  | 4   | 1  | 3 | 8 | 131  | 130  | 2   | 2  | 3 | 9 | 129  | 131  | 2   | 0  | 1 | 12 | 112  | 113  | 3   |
| 4  | 8 | 6 | 130  | 133  | 6   | 0  | 5  | 7 | 159  | 163  | 2   | 2  | 3 | 8 | 200  | 195  | 8   | 3  | 3 | 9 | 157  | 156  | 5   |    |   |    |      |      |     |
| 5  | 8 | 6 | 216  | 221  | 4   | 1  | 5  | 7 | 67   | 74   | 2   | 3  | 3 | 8 | 132  | 136  | 4   | 4  | 3 | 9 | 27   | 30   | 12  |    |   |    |      |      |     |