**The calculation of and for Ag2Te (hessite) in the range of 0< 2θ ≤ 130º (Cu *K*α1)**

1. **The calculation of**

Step 1: generate all the possible reflection indices *h* in the range of 0< 2θ ≤ 130º (Cu *K*α1) according to the unit cell parameters and space group (*P*21/*c*) of the hessite.

Step 2: calculate *d* values for all the reflection indices *h* generated in step 1 according to the unit cell parameters.

Step 3: calculate the atomic scattering factors *fi,h* of constitute elements (Ag and Te) for each *d* value obtained in step 2.

Step 4: generate the fractional coordinates of all atoms (8 Ag and 4 Te) in the unit cell according to the space group and independent atomic coordinates.

Step 5: calculate according to

Step 6: sum up over all reflections in the desired 2θ to get

The results of the calculations are given below. Note that the subscript *h* in the following table represents the index of only one reflection in a symmetrically equivalent group, and therefore the multiplicity *m* is incorporated in the calculation of . In the main text of this paper, the subscript *h* represents all possible reflection indices in a symmetrically equivalent group. Thus defined in the main text is equivalent to reported in the following table.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 2θ | *h* |  | Multiplicity |  | 2θUL |  |
| 13.095 | 1 0 0 | 62.64 | 2 | 7847.5392 |  |  |
| 19.766 | -1 0 2 | 79.74 | 2 | 12716.9352 |  |  |
| 23.132 | -1 1 1 | 6.74 | 4 | 181.7104 |  |  |
| 23.213 | 0 1 1 | 25.73 | 4 | 2648.1316 |  |  |
| 23.625 | -2 0 2 | 46.55 | 2 | 4333.805 |  |  |
| 23.858 | 1 1 0 | 44.52 | 4 | 7928.1216 |  |  |
| 23.94 | 0 0 2 | 23.2 | 2 | 1076.48 |  |  |
| 26.365 | 2 0 0 | 96.39 | 2 | 18582.0642 |  |  |
| 28.159 | -1 1 2 | 130.69 | 4 | 68319.5044 |  |  |
| 29.756 | -2 1 1 | 117.91 | 4 | 55611.0724 |  |  |
| 29.947 | 1 1 1 | 206.78 | 4 | 171031.8736 | 30 | 350277.2376 |
| 31.047 | -2 1 2 | 296.1 | 4 | 350700.84 |  |  |
| 31.293 | 0 1 2 | 107.54 | 4 | 46259.4064 |  |  |
| 32.935 | -3 0 2 | 12.18 | 2 | 296.7048 |  |  |
| 33.224 | 2 1 0 | 105.45 | 4 | 44478.81 |  |  |
| 33.399 | 1 0 2 | 52.18 | 2 | 5445.5048 |  |  |
| 36.647 | -2 1 3 | 80.5 | 4 | 25921 |  |  |
| 36.807 | -1 1 3 | 58.2 | 4 | 13548.96 |  |  |
| 38.754 | -3 1 2 | 225.2 | 4 | 202860.16 |  |  |
| 39.158 | 1 1 2 | 368.94 | 4 | 544466.8944 | 40 | 1584255.518 |
| 40.007 | 3 0 0 | 349.87 | 2 | 244818.0338 |  |  |
| 40.121 | -3 1 1 | 35.05 | 4 | 4914.01 |  |  |
| 40.152 | -2 0 4 | 343.28 | 2 | 235682.3168 |  |  |
| 40.34 | 0 2 0 | 177.53 | 2 | 63033.8018 |  |  |
| 40.367 | 2 1 1 | 93.42 | 4 | 34909.1856 |  |  |
| 41.238 | -3 1 3 | 230.43 | 4 | 212391.9396 |  |  |
| 41.67 | 0 1 3 | 128.36 | 4 | 65905.1584 |  |  |
| 42.161 | -1 2 1 | 193.94 | 4 | 150450.8944 |  |  |
| 42.208 | 0 2 1 | 247.46 | 4 | 244945.8064 |  |  |
| 42.222 | -3 0 4 | 103.52 | 2 | 21432.7808 |  |  |
| 42.59 | 1 2 0 | 4.78 | 4 | 91.3936 |  |  |
| 42.598 | -1 0 4 | 276.01 | 2 | 152363.0402 |  |  |
| 44.735 | -4 0 2 | 270.56 | 2 | 146405.4272 |  |  |
| 45.047 | 3 1 0 | 78.16 | 4 | 24435.9424 |  |  |
| 45.179 | -2 1 4 | 13.35 | 4 | 712.89 |  |  |
| 45.273 | 2 0 2 | 100.53 | 2 | 20212.5618 |  |  |
| 45.308 | -1 2 2 | 27.04 | 4 | 2924.6464 |  |  |
| 46.385 | -2 2 1 | 127.93 | 4 | 65464.3396 |  |  |
| 46.516 | 1 2 1 | 38.13 | 4 | 5815.5876 |  |  |
| 47.07 | -3 1 4 | 166.71 | 4 | 111168.8964 |  |  |
| 47.281 | -2 2 2 | 17.31 | 4 | 1198.5444 |  |  |
| 47.416 | -1 1 4 | 1.73 | 4 | 11.9716 |  |  |
| 47.453 | 0 2 2 | 2.62 | 4 | 27.4576 |  |  |
| 48.337 | -4 0 4 | 82.44 | 2 | 13592.7072 |  |  |
| 48.837 | 2 2 0 | 47.85 | 4 | 9158.49 |  |  |
| 49.013 | 0 0 4 | 147.85 | 2 | 43719.245 |  |  |
| 49.388 | -4 1 2 | 77.68 | 4 | 24136.7296 |  |  |
| 49.487 | -4 1 3 | 14.64 | 4 | 857.3184 |  |  |
| 49.888 | 2 1 2 | 10.27 | 4 | 421.8916 | 50 | 3485458.526 |
| 50.11 | 1 1 3 | 104.57 | 4 | 43739.5396 |  |  |
| 51.392 | -2 2 3 | 73.73 | 4 | 21744.4516 |  |  |
| 51.514 | -1 2 3 | 206.41 | 4 | 170420.3524 |  |  |
| 52.467 | -4 1 1 | 12.7 | 4 | 645.16 |  |  |
| 52.747 | 3 1 1 | 74.87 | 4 | 22422.0676 |  |  |
| 52.749 | -4 1 4 | 67.12 | 4 | 18020.3776 |  |  |
| 53.022 | -3 2 2 | 13.26 | 4 | 703.3104 |  |  |
| 53.34 | 1 2 2 | 20.91 | 4 | 1748.9124 |  |  |
| 53.384 | 0 1 4 | 0.14 | 4 | 0.0784 |  |  |
| 54.102 | -3 2 1 | 174.31 | 4 | 121535.9044 |  |  |
| 54.272 | 4 0 0 | 176.63 | 2 | 62396.3138 |  |  |
| 54.297 | 2 2 1 | 37.18 | 4 | 5529.4096 |  |  |
| 54.996 | -3 2 3 | 18.29 | 4 | 1338.0964 |  |  |
| 55.344 | 0 2 3 | 40.79 | 4 | 6655.2964 |  |  |
| 55.444 | -3 1 5 | 27.75 | 4 | 3080.25 |  |  |
| 55.636 | -2 1 5 | 33.43 | 4 | 4470.2596 |  |  |
| 57.524 | -5 0 4 | 260.14 | 2 | 135345.6392 |  |  |
| 58.031 | -5 0 2 | 35.8 | 2 | 2563.28 |  |  |
| 58.117 | 3 2 0 | 116.91 | 4 | 54671.7924 |  |  |
| 58.227 | -2 2 4 | 112.37 | 4 | 50508.0676 |  |  |
| 58.366 | 4 1 0 | 14.47 | 4 | 837.5236 |  |  |
| 58.422 | 1 0 4 | 169.12 | 2 | 57203.1488 |  |  |
| 58.628 | 3 0 2 | 119.62 | 2 | 28617.8888 |  |  |
| 58.803 | -4 1 5 | 27.92 | 4 | 3118.1056 |  |  |
| 59.358 | -1 1 5 | 68.45 | 4 | 18741.61 |  |  |
| 59.817 | -3 2 4 | 51.82 | 4 | 10741.2496 | 60 | 4332256.612 |
| 60.11 | -1 2 4 | 89.34 | 4 | 31926.5424 |  |  |
| 60.313 | -5 1 3 | 8.39 | 4 | 281.5684 |  |  |
| 61.077 | 2 1 3 | 5.16 | 4 | 106.5024 |  |  |
| 61.477 | -5 1 4 | 105.58 | 4 | 44588.5456 |  |  |
| 61.797 | -4 2 2 | 93.57 | 4 | 35021.3796 |  |  |
| 61.882 | -4 2 3 | 21.74 | 4 | 1890.5104 |  |  |
| 61.965 | -5 1 2 | 89.73 | 4 | 32205.8916 |  |  |
| 61.982 | -3 0 6 | 92.59 | 2 | 17145.8162 |  |  |
| 62.229 | 2 2 2 | 32.13 | 4 | 4129.3476 |  |  |
| 62.341 | 1 1 4 | 17.94 | 4 | 1287.3744 |  |  |
| 62.421 | 1 2 3 | 14.4 | 4 | 829.44 |  |  |
| 62.539 | 3 1 2 | 21.62 | 4 | 1869.6976 |  |  |
| 63.444 | -4 0 6 | 96.42 | 2 | 18593.6328 |  |  |
| 63.638 | -1 3 1 | 0.19 | 4 | 0.1444 |  |  |
| 63.674 | 0 3 1 | 47.18 | 4 | 8903.8096 |  |  |
| 63.869 | -2 0 6 | 117.49 | 2 | 27607.8002 |  |  |
| 63.961 | 1 3 0 | 15.3 | 4 | 936.36 |  |  |
| 64.477 | -4 2 1 | 304.52 | 4 | 370929.7216 |  |  |
| 64.723 | 3 2 1 | 98.27 | 4 | 38627.9716 |  |  |
| 64.725 | -4 2 4 | 22.17 | 4 | 1966.0356 |  |  |
| 65.285 | 0 2 4 | 69.03 | 4 | 19060.5636 |  |  |
| 65.372 | -5 1 5 | 24.17 | 4 | 2336.7556 |  |  |
| 65.776 | -3 1 6 | 13.44 | 4 | 722.5344 |  |  |
| 66.042 | -1 3 2 | 5.19 | 4 | 107.7444 |  |  |
| 66.242 | 0 1 5 | 121.56 | 4 | 59107.3344 |  |  |
| 66.313 | -5 1 1 | 11.58 | 4 | 536.3856 |  |  |
| 66.624 | 4 1 1 | 128.95 | 4 | 66512.41 |  |  |
| 66.885 | -2 3 1 | 154.89 | 4 | 95963.6484 |  |  |
| 66.988 | 1 3 1 | 273.41 | 4 | 299012.1124 |  |  |
| 67.115 | -3 2 5 | 20.37 | 4 | 1659.7476 |  |  |
| 67.193 | -4 1 6 | 238.62 | 4 | 227758.0176 |  |  |
| 67.288 | -2 2 5 | 305.2 | 4 | 372588.16 |  |  |
| 67.594 | -2 3 2 | 50.62 | 4 | 10249.5376 |  |  |
| 67.605 | -2 1 6 | 63.77 | 4 | 16266.4516 |  |  |
| 67.731 | 0 3 2 | 32.24 | 4 | 4157.6704 |  |  |
| 68.137 | -5 0 6 | 144.59 | 2 | 41812.5362 |  |  |
| 68.84 | 2 3 0 | 11.96 | 4 | 572.1664 |  |  |
| 68.956 | -1 0 6 | 11.17 | 2 | 249.5378 |  |  |
| 69.075 | -6 0 4 | 34.12 | 2 | 2328.3488 |  |  |
| 69.518 | 5 0 0 | 46.47 | 2 | 4318.9218 |  |  |
| 69.748 | 4 2 0 | 53.17 | 4 | 11308.1956 | 70 | 6207733.484 |
| 70.145 | -4 2 5 | 59.45 | 4 | 14137.21 |  |  |
| 70.159 | 2 0 4 | 313.36 | 2 | 196388.9792 |  |  |
| 70.651 | -1 2 5 | 55.18 | 4 | 12179.3296 |  |  |
| 70.928 | -2 3 3 | 99.68 | 4 | 39744.4096 |  |  |
| 71.029 | -1 3 3 | 96.89 | 4 | 37550.6884 |  |  |
| 71.523 | -5 2 3 | 8.09 | 4 | 261.7924 |  |  |
| 71.763 | -5 1 6 | 39.57 | 4 | 6263.1396 |  |  |
| 72.224 | 2 2 3 | 287.39 | 4 | 330372.0484 |  |  |
| 72.286 | -3 3 2 | 48.02 | 4 | 9223.6816 |  |  |
| 72.552 | 1 3 2 | 62.98 | 4 | 15865.9216 |  |  |
| 72.564 | -1 1 6 | 262.02 | 4 | 274617.9216 |  |  |
| 72.592 | -5 2 4 | 89.14 | 4 | 31783.7584 |  |  |
| 72.681 | -6 1 4 | 166.09 | 4 | 110343.5524 |  |  |
| 72.751 | -6 0 2 | 113.43 | 2 | 25732.7298 |  |  |
| 73.042 | -5 2 2 | 8.44 | 4 | 284.9344 |  |  |
| 73.114 | 5 1 0 | 216.59 | 4 | 187644.9124 |  |  |
| 73.195 | -3 3 1 | 43.49 | 4 | 7565.5204 |  |  |
| 73.208 | -6 1 3 | 182.65 | 4 | 133444.09 |  |  |
| 73.36 | 2 3 1 | 121.75 | 4 | 59292.25 |  |  |
| 73.389 | 1 2 4 | 53.14 | 4 | 11295.4384 |  |  |
| 73.414 | 4 0 2 | 118.08 | 2 | 27885.7728 |  |  |
| 73.572 | 3 2 2 | 44.59 | 4 | 7953.0724 |  |  |
| 73.742 | 2 1 4 | 55.35 | 4 | 12254.49 |  |  |
| 73.954 | -3 3 3 | 319.44 | 4 | 408167.6544 |  |  |
| 74.101 | 3 1 3 | 23.98 | 4 | 2300.1616 |  |  |
| 74.251 | 0 3 3 | 174.87 | 4 | 122318.0676 |  |  |
| 74.723 | -6 1 5 | 4.79 | 4 | 91.7764 |  |  |
| 75.777 | -6 0 6 | 250.69 | 2 | 125690.9522 |  |  |
| 75.872 | 1 1 5 | 44.54 | 4 | 7935.2464 |  |  |
| 76.208 | -5 2 5 | 287.2 | 4 | 329935.36 |  |  |
| 76.285 | -6 1 2 | 145.84 | 4 | 85077.2224 |  |  |
| 76.587 | -3 2 6 | 32.89 | 4 | 4327.0084 |  |  |
| 76.647 | 3 3 0 | 6.34 | 4 | 160.7824 |  |  |
| 76.743 | -2 3 4 | 10.09 | 4 | 407.2324 |  |  |
| 76.938 | 4 1 2 | 211.76 | 4 | 179369.1904 |  |  |
| 76.953 | 0 0 6 | 5.3 | 2 | 56.18 |  |  |
| 77.024 | 0 2 5 | 41.81 | 4 | 6992.3044 |  |  |
| 77.091 | -5 2 1 | 59.08 | 4 | 13961.7856 |  |  |
| 77.384 | 4 2 1 | 47.22 | 4 | 8918.9136 |  |  |
| 77.627 | -4 1 7 | 152.88 | 4 | 93489.1776 |  |  |
| 77.855 | -3 1 7 | 44.75 | 4 | 8010.25 |  |  |
| 77.919 | -4 2 6 | 44.15 | 4 | 7796.89 |  |  |
| 78.139 | -3 3 4 | 31.15 | 4 | 3881.29 |  |  |
| 78.308 | -2 2 6 | 38.5 | 4 | 5929 |  |  |
| 78.399 | -1 3 4 | 2.94 | 4 | 34.5744 |  |  |
| 79.266 | -6 1 6 | 22.08 | 4 | 1950.1056 |  |  |
| 79.9 | -4 3 2 | 7.8 | 4 | 243.36 |  |  |
| 79.976 | -4 3 3 | 36.66 | 4 | 5375.8224 | 80 | 9182239.436 |
| 80.287 | 2 3 2 | 19.64 | 4 | 1542.9184 |  |  |
| 80.427 | 0 1 6 | 130.2 | 4 | 67808.16 |  |  |
| 80.436 | -5 1 7 | 117.71 | 4 | 55422.5764 |  |  |
| 80.459 | 1 3 3 | 145.1 | 4 | 84216.04 |  |  |
| 81.112 | -2 1 7 | 39.54 | 4 | 6253.6464 |  |  |
| 81.821 | -6 1 1 | 2.61 | 4 | 27.2484 |  |  |
| 82.174 | 5 1 1 | 144.2 | 4 | 83174.56 |  |  |
| 82.264 | -5 2 6 | 45.95 | 4 | 8445.61 |  |  |
| 82.319 | -4 3 1 | 15.9 | 4 | 1011.24 |  |  |
| 82.544 | 3 3 1 | 126.33 | 4 | 63837.0756 |  |  |
| 82.545 | -4 3 4 | 12.61 | 4 | 636.0484 |  |  |
| 82.801 | -7 0 4 | 14.01 | 2 | 392.5602 |  |  |
| 83.032 | -1 2 6 | 0.77 | 4 | 2.3716 |  |  |
| 83.057 | 0 3 4 | 0.72 | 4 | 2.0736 |  |  |
| 83.145 | -6 2 4 | 2.3 | 4 | 21.16 |  |  |
| 83.562 | 5 2 0 | 27.45 | 4 | 3014.01 |  |  |
| 83.652 | -6 2 3 | 68.23 | 4 | 18621.3316 |  |  |
| 84.079 | 3 0 4 | 28.94 | 2 | 1675.0472 |  |  |
| 84.167 | 2 2 4 | 109.83 | 4 | 48250.5156 |  |  |
| 84.514 | 3 2 3 | 67.02 | 4 | 17966.7216 |  |  |
| 84.742 | -3 3 5 | 39.77 | 4 | 6326.6116 |  |  |
| 84.901 | -2 3 5 | 56.66 | 4 | 12841.4224 |  |  |
| 85.116 | -6 2 5 | 142.14 | 4 | 80815.1184 |  |  |
| 86.159 | -7 0 6 | 89.57 | 2 | 16045.5698 |  |  |
| 86.215 | -6 1 7 | 52.48 | 4 | 11016.6016 |  |  |
| 86.223 | -7 1 4 | 181.26 | 4 | 131420.7504 |  |  |
| 86.23 | 1 2 5 | 146.11 | 4 | 85392.5284 |  |  |
| 86.338 | 6 0 0 | 102.42 | 2 | 20979.7128 |  |  |
| 86.632 | -6 2 2 | 52.84 | 4 | 11168.2624 |  |  |
| 86.662 | -7 1 5 | 66.05 | 4 | 17450.41 |  |  |
| 86.713 | -4 0 8 | 83.19 | 2 | 13841.1522 |  |  |
| 87.196 | 4 3 0 | 15.03 | 4 | 903.6036 |  |  |
| 87.199 | 0 4 0 | 223.93 | 2 | 100289.2898 |  |  |
| 87.268 | 4 2 2 | 49.86 | 4 | 9944.0784 |  |  |
| 87.328 | -1 1 7 | 146.06 | 4 | 85334.0944 |  |  |
| 87.494 | 3 1 4 | 106.7 | 4 | 45539.56 |  |  |
| 87.569 | -4 3 5 | 38.59 | 4 | 5956.7524 |  |  |
| 87.685 | 1 0 6 | 49.79 | 2 | 4958.0882 |  |  |
| 87.941 | -4 2 7 | 10.95 | 4 | 479.61 |  |  |
| 87.95 | -5 0 8 | 63.06 | 2 | 7953.1272 |  |  |
| 88.046 | -1 3 5 | 95.98 | 4 | 36848.6416 |  |  |
| 88.092 | 2 1 5 | 15.75 | 4 | 992.25 |  |  |
| 88.163 | -3 2 7 | 80.5 | 4 | 25921 |  |  |
| 88.251 | -7 1 3 | 59.03 | 4 | 13938.1636 |  |  |
| 88.401 | -1 4 1 | 103.67 | 4 | 42989.8756 |  |  |
| 88.432 | 0 4 1 | 134.09 | 4 | 71920.5124 |  |  |
| 88.458 | -3 0 8 | 271.06 | 2 | 146947.0472 |  |  |
| 88.69 | 1 4 0 | 40 | 4 | 6400 |  |  |
| 88.871 | -5 3 3 | 26.33 | 4 | 2773.0756 |  |  |
| 89.299 | 4 1 3 | 25.39 | 4 | 2578.6084 |  |  |
| 89.335 | -7 0 2 | 233.4 | 2 | 108951.12 |  |  |
| 89.538 | 2 3 3 | 16.59 | 4 | 1100.9124 |  |  |
| 89.547 | -6 2 6 | 90.91 | 4 | 33058.5124 |  |  |
| 89.568 | -7 1 6 | 83.54 | 4 | 27915.7264 |  |  |
| 89.747 | 6 1 0 | 15.34 | 4 | 941.2624 |  |  |
| 89.889 | -5 3 4 | 0.93 | 4 | 3.4596 | 90 | 10836496.86 |
| 90.097 | 5 0 2 | 59.54 | 2 | 7090.0232 |  |  |
| 90.12 | -4 1 8 | 64.58 | 4 | 16682.3056 |  |  |
| 90.318 | -5 3 2 | 19.8 | 4 | 1568.16 |  |  |
| 90.576 | -1 4 2 | 29.24 | 4 | 3419.9104 |  |  |
| 90.651 | 1 3 4 | 8.68 | 4 | 301.3696 |  |  |
| 90.69 | 0 2 6 | 4.25 | 4 | 72.25 |  |  |
| 90.699 | -5 2 7 | 2.54 | 4 | 25.8064 |  |  |
| 90.826 | 3 3 2 | 11.05 | 4 | 488.41 |  |  |
| 91.091 | 1 1 6 | 94.25 | 4 | 35532.25 |  |  |
| 91.349 | -2 4 1 | 99.23 | 4 | 39386.3716 |  |  |
| 91.357 | -5 1 8 | 187.02 | 4 | 139905.9216 |  |  |
| 91.366 | -2 2 7 | 33.92 | 4 | 4602.2656 |  |  |
| 91.444 | 1 4 1 | 39.86 | 4 | 6355.2784 |  |  |
| 91.865 | -3 1 8 | 42.2 | 4 | 7123.36 |  |  |
| 92.003 | -2 4 2 | 20.75 | 4 | 1722.25 |  |  |
| 92.068 | -6 2 1 | 28.17 | 4 | 3174.1956 |  |  |
| 92.13 | 0 4 2 | 19.51 | 4 | 1522.5604 |  |  |
| 92.167 | -6 0 8 | 119.22 | 2 | 28426.8168 |  |  |
| 92.417 | 5 2 1 | 34.48 | 4 | 4755.4816 |  |  |
| 92.742 | -7 1 2 | 26.8 | 4 | 2872.96 |  |  |
| 93.161 | 2 4 0 | 26.19 | 4 | 2743.6644 |  |  |
| 93.184 | -2 0 8 | 30.74 | 2 | 1889.8952 |  |  |
| 93.373 | -5 3 5 | 35.18 | 4 | 4950.5296 |  |  |
| 93.505 | 5 1 2 | 78.74 | 4 | 24799.9504 |  |  |
| 93.742 | -3 3 6 | 13.79 | 4 | 760.6564 |  |  |
| 94.168 | 0 3 5 | 183.1 | 4 | 134102.44 |  |  |
| 94.234 | -5 3 1 | 18.27 | 4 | 1335.1716 |  |  |
| 94.52 | 4 3 1 | 189.27 | 4 | 143292.5316 |  |  |
| 94.941 | -7 1 7 | 72.82 | 4 | 21211.0096 |  |  |
| 95.045 | -4 3 6 | 44.14 | 4 | 7793.3584 |  |  |
| 95.127 | -2 4 3 | 32.87 | 4 | 4321.7476 |  |  |
| 95.223 | -1 4 3 | 121.69 | 4 | 59233.8244 |  |  |
| 95.427 | -2 3 6 | 9.31 | 4 | 346.7044 |  |  |
| 95.581 | -6 1 8 | 40.85 | 4 | 6674.89 |  |  |
| 96.422 | -3 4 2 | 7.76 | 4 | 240.8704 |  |  |
| 96.45 | -6 2 7 | 65.6 | 4 | 17213.44 |  |  |
| 96.457 | -7 2 4 | 2.07 | 4 | 17.1396 |  |  |
| 96.505 | 0 1 7 | 16.1 | 4 | 1036.84 |  |  |
| 96.603 | -2 1 8 | 56.58 | 4 | 12805.1856 |  |  |
| 96.678 | 1 4 2 | 18.21 | 4 | 1326.4164 |  |  |
| 96.899 | -7 2 5 | 74.15 | 4 | 21992.89 |  |  |
| 97.296 | -3 4 1 | 92.31 | 4 | 34084.5444 |  |  |
| 97.456 | 2 4 1 | 17.53 | 4 | 1229.2036 |  |  |
| 97.569 | -1 2 7 | 68.71 | 4 | 18884.2564 |  |  |
| 97.737 | 3 2 4 | 23.17 | 4 | 2147.3956 |  |  |
| 98.031 | -3 4 3 | 17.52 | 4 | 1227.8016 |  |  |
| 98.32 | 0 4 3 | 37.15 | 4 | 5520.49 |  |  |
| 98.34 | 2 2 5 | 90.62 | 4 | 32847.9376 |  |  |
| 98.5 | -7 2 3 | 27.89 | 4 | 3111.4084 |  |  |
| 99.12 | -8 0 4 | 59.64 | 2 | 7113.8592 |  |  |
| 99.359 | -5 3 6 | 22.54 | 4 | 2032.2064 |  |  |
| 99.404 | -7 0 8 | 94.05 | 2 | 17690.805 |  |  |
| 99.423 | -8 0 6 | 28.33 | 2 | 1605.1778 |  |  |
| 99.561 | 4 2 3 | 86.65 | 4 | 30032.89 |  |  |
| 99.743 | -7 1 1 | 53.95 | 4 | 11642.41 |  |  |
| 99.834 | -7 2 6 | 43.46 | 4 | 7555.0864 | 100 | 11786339.44 |
| 100.016 | 6 2 0 | 35.95 | 4 | 5169.61 |  |  |
| 100.132 | -1 3 6 | 50.35 | 4 | 10140.49 |  |  |
| 100.162 | 6 1 1 | 36.57 | 4 | 5349.4596 |  |  |
| 100.246 | -6 3 4 | 36.05 | 4 | 5198.41 |  |  |
| 100.395 | -4 2 8 | 22.35 | 4 | 1998.09 |  |  |
| 100.667 | 4 0 4 | 24.79 | 2 | 1229.0882 |  |  |
| 100.667 | 5 3 0 | 36.92 | 4 | 5452.3456 |  |  |
| 100.671 | 3 4 0 | 160.19 | 4 | 102643.3444 |  |  |
| 100.759 | -6 3 3 | 277.59 | 4 | 308224.8324 |  |  |
| 100.766 | -2 4 4 | 162.46 | 4 | 105573.0064 |  |  |
| 100.952 | -1 0 8 | 27.35 | 2 | 1496.045 |  |  |
| 101.28 | 2 3 4 | 1.93 | 4 | 14.8996 |  |  |
| 101.359 | 2 0 6 | 39.54 | 2 | 3126.8232 |  |  |
| 101.384 | 1 2 6 | 20.48 | 4 | 1677.7216 |  |  |
| 101.481 | -8 1 5 | 21.36 | 4 | 1824.9984 |  |  |
| 101.632 | 3 3 3 | 35.95 | 4 | 5169.61 |  |  |
| 101.655 | -5 2 8 | 31.18 | 4 | 3888.7696 |  |  |
| 102.157 | -3 4 4 | 29.98 | 4 | 3595.2016 |  |  |
| 102.174 | -3 2 8 | 99.33 | 4 | 39465.7956 |  |  |
| 102.245 | -6 3 5 | 3.37 | 4 | 45.4276 |  |  |
| 102.417 | -1 4 4 | 132.25 | 4 | 69960.25 |  |  |
| 102.588 | -8 1 4 | 93.82 | 4 | 35208.7696 |  |  |
| 102.876 | -7 1 8 | 16.1 | 4 | 1036.84 |  |  |
| 102.895 | -8 1 6 | 49.83 | 4 | 9932.1156 |  |  |
| 103.073 | -7 2 2 | 84.11 | 4 | 28297.9684 |  |  |
| 103.269 | 3 1 5 | 155.46 | 4 | 96671.2464 |  |  |
| 103.384 | 1 3 5 | 78.19 | 4 | 24454.7044 |  |  |
| 103.797 | -6 3 2 | 33.58 | 4 | 4510.4656 |  |  |
| 103.856 | 5 2 2 | 16.21 | 4 | 1051.0564 |  |  |
| 103.931 | -4 4 2 | 126.62 | 4 | 64130.4976 |  |  |
| 104.008 | -4 4 3 | 14.54 | 4 | 845.6464 |  |  |
| 104.155 | 4 1 4 | 70.92 | 4 | 20118.5856 |  |  |
| 104.324 | 2 4 2 | 53.24 | 4 | 11337.9904 |  |  |
| 104.444 | -1 1 8 | 43.22 | 4 | 7471.8736 |  |  |
| 104.452 | 4 3 2 | 41.07 | 4 | 6746.9796 |  |  |
| 104.5 | 1 4 3 | 26.9 | 4 | 2894.44 |  |  |
| 104.857 | 2 1 6 | 137.94 | 4 | 76109.7744 |  |  |
| 104.863 | -5 1 9 | 13.14 | 4 | 690.6384 |  |  |
| 105.147 | -4 3 7 | 232.41 | 4 | 216057.6324 |  |  |
| 105.158 | -4 1 9 | 9.48 | 4 | 359.4816 |  |  |
| 105.336 | -7 2 7 | 9.25 | 4 | 342.25 |  |  |
| 105.377 | -3 3 7 | 83.56 | 4 | 27929.0944 |  |  |
| 105.913 | 7 0 0 | 106.83 | 2 | 22825.2978 |  |  |
| 105.997 | -6 2 8 | 43.87 | 4 | 7698.3076 |  |  |
| 106.252 | -8 1 3 | 24.11 | 4 | 2325.1684 |  |  |
| 106.408 | -4 4 1 | 185.19 | 4 | 137181.3444 |  |  |
| 106.639 | 3 4 1 | 56.24 | 4 | 12651.7504 |  |  |
| 106.641 | -4 4 4 | 43.33 | 4 | 7509.9556 |  |  |
| 106.817 | -6 3 6 | 4.64 | 4 | 86.1184 |  |  |
| 106.875 | -8 1 7 | 127.2 | 4 | 64719.36 |  |  |
| 106.955 | 0 2 7 | 127.3 | 4 | 64821.16 |  |  |
| 107.057 | -2 2 8 | 20.42 | 4 | 1667.9056 |  |  |
| 107.172 | 0 4 4 | 51.7 | 4 | 10691.56 |  |  |
| 107.546 | 5 1 3 | 35.33 | 4 | 4992.8356 |  |  |
| 107.669 | -6 1 9 | 1.54 | 4 | 9.4864 |  |  |
| 108.015 | 0 3 6 | 33.54 | 4 | 4499.7264 |  |  |
| 108.025 | -5 3 7 | 177.14 | 4 | 125514.3184 |  |  |
| 108.571 | -3 1 9 | 1.8 | 4 | 12.96 |  |  |
| 108.727 | -2 3 7 | 54.78 | 4 | 12003.3936 |  |  |
| 108.934 | -3 4 5 | 3.1 | 4 | 38.44 |  |  |
| 108.977 | 1 1 7 | 0.15 | 4 | 0.09 |  |  |
| 108.986 | -8 0 2 | 162.61 | 2 | 52884.0242 |  |  |
| 109.102 | -2 4 5 | 188.67 | 4 | 142385.4756 |  |  |
| 109.47 | -6 3 1 | 8.6 | 4 | 295.84 |  |  |
| 109.489 | 7 1 0 | 64.97 | 4 | 16884.4036 |  |  |
| 109.84 | 5 3 1 | 220.65 | 4 | 194745.69 |  |  |
| 109.929 | 6 0 2 | 228.57 | 2 | 104488.4898 |  |  |
| 109.937 | -8 0 8 | 17.73 | 2 | 628.7058 | 110 | 14095343.51 |
| 110.339 | -7 2 1 | 241.25 | 4 | 232806.25 |  |  |
| 110.779 | 6 2 1 | 55.4 | 4 | 12276.64 |  |  |
| 111.543 | 4 4 0 | 98.35 | 4 | 38690.89 |  |  |
| 111.945 | -4 4 5 | 59.34 | 4 | 14084.9424 |  |  |
| 112.114 | 0 0 8 | 277.74 | 2 | 154279.0152 |  |  |
| 112.172 | -8 2 5 | 136.97 | 4 | 75043.1236 |  |  |
| 112.459 | -1 4 5 | 17.66 | 4 | 1247.5024 |  |  |
| 112.631 | -8 1 2 | 28.24 | 4 | 3189.9904 |  |  |
| 113.346 | -8 2 4 | 20.33 | 4 | 1653.2356 |  |  |
| 113.355 | -5 4 3 | 2.11 | 4 | 17.8084 |  |  |
| 113.597 | 6 1 2 | 5.05 | 4 | 102.01 |  |  |
| 113.605 | -8 1 8 | 228.35 | 4 | 208574.89 |  |  |
| 113.652 | -7 2 8 | 29.45 | 4 | 3469.21 |  |  |
| 113.672 | -8 2 6 | 2.26 | 4 | 20.4304 |  |  |
| 113.738 | -7 1 9 | 28.92 | 4 | 3345.4656 |  |  |
| 114.07 | 3 2 5 | 17.43 | 4 | 1215.2196 |  |  |
| 114.083 | 2 4 3 | 181.03 | 4 | 131087.4436 |  |  |
| 114.177 | -6 3 7 | 96.44 | 4 | 37202.6944 |  |  |
| 114.185 | -7 3 4 | 35.4 | 4 | 5012.64 |  |  |
| 114.468 | -5 4 4 | 132.63 | 4 | 70362.8676 |  |  |
| 114.667 | -7 3 5 | 105.91 | 4 | 44867.7124 |  |  |
| 114.941 | -5 4 2 | 21.1 | 4 | 1780.84 |  |  |
| 115.016 | 4 2 4 | 3.4 | 4 | 46.24 |  |  |
| 115.308 | 1 4 4 | 91.32 | 4 | 33357.3696 |  |  |
| 115.308 | -2 1 9 | 66.64 | 4 | 17763.5584 |  |  |
| 115.326 | -1 2 8 | 20.54 | 4 | 1687.5664 |  |  |
| 115.401 | -1 3 7 | 227.1 | 4 | 206297.64 |  |  |
| 115.502 | 3 4 2 | 55.4 | 4 | 12276.64 |  |  |
| 115.585 | 3 3 4 | 21.36 | 4 | 1824.9984 |  |  |
| 115.769 | 2 2 6 | 13.52 | 4 | 731.1616 |  |  |
| 115.775 | -5 2 9 | 75.9 | 4 | 23043.24 |  |  |
| 115.842 | 0 1 8 | 29.96 | 4 | 3590.4064 |  |  |
| 116.093 | -4 2 9 | 198.39 | 4 | 157434.3684 |  |  |
| 116.249 | 2 3 5 | 15.52 | 4 | 963.4816 |  |  |
| 116.426 | -7 3 3 | 82.85 | 4 | 27456.49 |  |  |
| 116.515 | -9 0 6 | 277.99 | 2 | 154556.8802 |  |  |
| 117.271 | -8 2 3 | 122.97 | 4 | 60486.4836 |  |  |
| 117.602 | 4 3 3 | 35.4 | 4 | 5012.64 |  |  |
| 117.906 | -7 3 6 | 16.56 | 4 | 1096.9344 |  |  |
| 117.945 | -8 2 7 | 60.85 | 4 | 14810.89 |  |  |
| 118.109 | 6 3 0 | 6.06 | 4 | 146.8944 |  |  |
| 118.223 | -5 0 10 | 1.79 | 2 | 6.4082 |  |  |
| 118.357 | -5 4 5 | 180.9 | 4 | 130899.24 |  |  |
| 118.533 | -4 3 8 | 23.05 | 4 | 2125.21 |  |  |
| 118.673 | 5 2 3 | 196.15 | 4 | 153899.29 |  |  |
| 118.776 | -3 4 6 | 45.26 | 4 | 8193.8704 |  |  |
| 118.807 | -6 2 9 | 72.83 | 4 | 21216.8356 |  |  |
| 119.099 | 3 0 6 | 57.73 | 2 | 6665.5058 |  |  |
| 119.262 | 0 4 5 | 40.46 | 4 | 6548.0464 |  |  |
| 119.337 | -5 4 1 | 59.56 | 4 | 14189.5744 |  |  |
| 119.562 | -6 0 10 | 41.17 | 2 | 3389.9378 |  |  |
| 119.626 | -9 0 4 | 46.26 | 2 | 4279.9752 |  |  |
| 119.644 | 1 3 6 | 3.2 | 4 | 40.96 |  |  |
| 119.665 | 4 4 1 | 20.65 | 4 | 1705.69 |  |  |
| 119.79 | -3 2 9 | 171.01 | 4 | 116977.6804 |  |  |
| 119.95 | -5 3 8 | 34.6 | 4 | 4788.64 | 120 | 16333185.08 |
| 120.234 | 1 2 7 | 150.68 | 4 | 90817.8496 |  |  |
| 120.269 | -4 4 6 | 37.44 | 4 | 5607.0144 |  |  |
| 120.294 | -4 0 10 | 175.71 | 2 | 61748.0082 |  |  |
| 120.39 | -9 1 6 | 39.82 | 4 | 6342.5296 |  |  |
| 120.471 | -1 5 1 | 8 | 4 | 256 |  |  |
| 120.508 | 0 5 1 | 32.14 | 4 | 4131.9184 |  |  |
| 120.538 | -3 3 8 | 1.26 | 4 | 6.3504 |  |  |
| 120.552 | -9 1 5 | 32.06 | 4 | 4111.3744 |  |  |
| 120.711 | -2 4 6 | 64.91 | 4 | 16853.2324 |  |  |
| 120.795 | 7 2 0 | 34.01 | 4 | 4626.7204 |  |  |
| 120.807 | 1 5 0 | 34.63 | 4 | 4796.9476 |  |  |
| 121.562 | -7 3 2 | 17.58 | 4 | 1236.2256 |  |  |
| 121.692 | 5 0 4 | 181.19 | 2 | 65659.6322 |  |  |
| 122.164 | -5 1 10 | 87.52 | 4 | 30639.0016 |  |  |
| 122.19 | -8 1 1 | 35.71 | 4 | 5100.8164 |  |  |
| 122.46 | 5 3 2 | 28.77 | 4 | 3310.8516 |  |  |
| 122.754 | 7 1 1 | 39.79 | 4 | 6332.9764 |  |  |
| 122.979 | 4 1 5 | 13.37 | 4 | 715.0276 |  |  |
| 123.029 | -1 5 2 | 76.31 | 4 | 23292.8644 |  |  |
| 123.077 | 3 1 6 | 167.57 | 4 | 112318.8196 |  |  |
| 123.124 | -9 1 7 | 0.81 | 4 | 2.6244 |  |  |
| 123.56 | -6 1 10 | 103.62 | 4 | 42948.4176 |  |  |
| 123.614 | -8 1 9 | 59.75 | 4 | 14280.25 |  |  |
| 123.627 | -9 1 4 | 59.33 | 4 | 14080.1956 |  |  |
| 123.956 | -2 5 1 | 24.65 | 4 | 2430.49 |  |  |
| 124.071 | 1 5 1 | 42.58 | 4 | 7252.2256 |  |  |
| 124.174 | -7 3 7 | 111.46 | 4 | 49693.3264 |  |  |
| 124.272 | -8 2 2 | 57.76 | 4 | 13344.8704 |  |  |
| 124.325 | -4 1 10 | 71.15 | 4 | 20249.29 |  |  |
| 124.46 | -7 0 10 | 238.84 | 2 | 114089.0912 |  |  |
| 124.747 | -2 5 2 | 193.26 | 4 | 149397.7104 |  |  |
| 124.791 | -9 0 8 | 14.19 | 2 | 402.7122 |  |  |
| 124.902 | 0 5 2 | 74.89 | 4 | 22434.0484 |  |  |
| 124.947 | -6 3 8 | 4.72 | 4 | 89.1136 |  |  |
| 125.355 | 6 2 2 | 86.8 | 4 | 30136.96 |  |  |
| 125.362 | -5 4 6 | 82.76 | 4 | 27396.8704 |  |  |
| 125.364 | -8 2 8 | 2.46 | 4 | 24.2064 |  |  |
| 125.513 | -7 2 9 | 228.72 | 4 | 209251.3536 |  |  |
| 125.789 | 5 1 4 | 99.38 | 4 | 39505.5376 |  |  |
| 126.015 | -3 0 10 | 41.84 | 2 | 3501.1712 |  |  |
| 126.05 | -1 1 9 | 8.48 | 4 | 287.6416 |  |  |
| 126.076 | 0 3 7 | 14.77 | 4 | 872.6116 |  |  |
| 126.094 | 2 1 7 | 61.92 | 4 | 15336.3456 |  |  |
| 126.169 | 2 5 0 | 65.78 | 4 | 17308.0336 |  |  |
| 126.196 | -2 3 8 | 9.59 | 4 | 367.8724 |  |  |
| 126.302 | -1 4 6 | 12.19 | 4 | 594.3844 |  |  |
| 126.441 | -6 4 4 | 30.74 | 4 | 3779.7904 |  |  |
| 126.958 | 5 4 0 | 10.93 | 4 | 477.8596 |  |  |
| 127.07 | -6 4 3 | 46.21 | 4 | 8541.4564 |  |  |
| 127.288 | -2 2 9 | 65.63 | 4 | 17229.1876 |  |  |
| 127.714 | 2 4 4 | 167.17 | 4 | 111783.2356 |  |  |
| 127.896 | 0 2 8 | 102.96 | 4 | 42403.0464 |  |  |
| 127.945 | 1 0 8 | 85.15 | 2 | 14501.045 |  |  |
| 128.152 | 3 4 3 | 33.28 | 4 | 4430.2336 |  |  |
| 128.637 | -2 5 3 | 1.6 | 4 | 10.24 |  |  |
| 128.703 | -7 1 10 | 8.5 | 4 | 289 |  |  |
| 128.759 | -1 5 3 | 40.96 | 4 | 6710.8864 |  |  |
| 128.918 | -6 4 5 | 80.85 | 4 | 26146.89 |  |  |
| 129.053 | -9 1 8 | 51.03 | 4 | 10416.2436 |  |  |
| 129.96 | -9 1 3 | 83.51 | 4 | 27895.6804 | 130 | 17850981.39 |
| 130.151 | -7 3 1 | 89.85 | 4 | 32292.09 |  |  |
| 130.306 | -3 5 2 | 159.73 | 4 | 102054.6916 |  |  |
| 130.349 | -3 1 10 | 91.33 | 4 | 33364.6756 |  |  |
| 130.361 | 1 4 5 | 94.8 | 4 | 35948.16 |  |  |
| 130.639 | 1 5 2 | 254.49 | 4 | 259060.6404 |  |  |
| 130.693 | 6 3 1 | 71.57 | 4 | 20489.0596 |  |  |
| 130.89 | -6 4 2 | 44.56 | 4 | 7942.3744 |  |  |
| 131.454 | -3 5 1 | 7.67 | 4 | 235.3156 |  |  |
| 131.624 | 8 0 0 | 49.85 | 2 | 4970.045 |  |  |
| 131.666 | 2 5 1 | 12.47 | 4 | 622.0036 |  |  |
| 131.735 | 4 4 2 | 53.24 | 4 | 11337.9904 |  |  |
| 131.85 | 6 1 3 | 19.89 | 4 | 1582.4484 |  |  |
| 132.404 | 1 1 8 | 3.03 | 4 | 36.7236 |  |  |
| 132.424 | -8 3 5 | 35.03 | 4 | 4908.4036 |  |  |
| 132.433 | -3 5 3 | 54.62 | 4 | 11933.3776 |  |  |
| 132.642 | -4 4 7 | 0.39 | 4 | 0.6084 |  |  |
| 132.821 | 0 5 3 | 28.96 | 4 | 3354.7264 |  |  |
| 132.945 | -3 4 7 | 49.85 | 4 | 9940.09 |  |  |
| 133.174 | -9 2 6 | 103.74 | 4 | 43047.9504 |  |  |
| 133.366 | -9 2 5 | 156.26 | 4 | 97668.7504 |  |  |
| 133.655 | -8 0 10 | 105.12 | 2 | 22100.4288 |  |  |
| 133.909 | -8 3 4 | 0.45 | 4 | 0.81 |  |  |
| 134.299 | -7 3 8 | 12.37 | 4 | 612.0676 |  |  |
| 134.325 | -8 3 6 | 19.04 | 4 | 1450.0864 |  |  |
| 134.837 | 3 3 5 | 249.55 | 4 | 249100.81 |  |  |
| 134.865 | -6 4 6 | 133.08 | 4 | 70841.1456 |  |  |
| 135.291 | -5 2 10 | 5.4 | 4 | 116.64 |  |  |
| 135.322 | -8 2 1 | 50.42 | 4 | 10168.7056 |  |  |
| 135.585 | -9 0 2 | 102.75 | 2 | 21115.125 |  |  |
| 136.003 | 7 2 1 | 0.49 | 4 | 0.9604 |  |  |
| 136.063 | 4 3 4 | 11.45 | 4 | 524.41 |  |  |
| 136.07 | 3 5 0 | 54.66 | 4 | 11950.8624 |  |  |
| 136.204 | -2 5 4 | 3.21 | 4 | 41.2164 |  |  |
| 136.276 | 4 2 5 | 22.68 | 4 | 2057.5296 |  |  |
| 136.349 | -2 0 10 | 8.38 | 2 | 140.4488 |  |  |
| 136.359 | 8 1 0 | 190.95 | 4 | 145847.61 |  |  |
| 136.395 | 3 2 6 | 27.26 | 4 | 2972.4304 |  |  |
| 136.451 | -9 2 7 | 135.92 | 4 | 73896.9856 |  |  |
| 136.469 | -1 3 8 | 15.1 | 4 | 912.04 |  |  |
| 136.501 | 0 4 6 | 0.2 | 4 | 0.16 |  |  |
| 136.514 | -5 4 7 | 4.33 | 4 | 74.9956 |  |  |
| 136.983 | -6 2 10 | 25.45 | 4 | 2590.81 |  |  |
| 137.048 | -8 2 9 | 6.57 | 4 | 172.6596 |  |  |
| 137.052 | 2 3 6 | 31.44 | 4 | 3953.8944 |  |  |
| 137.056 | 7 0 2 | 49.74 | 2 | 4948.1352 |  |  |
| 137.06 | -5 3 9 | 19.79 | 4 | 1566.5764 |  |  |
| 137.064 | -9 2 4 | 11.47 | 4 | 526.2436 |  |  |
| 137.481 | -4 3 9 | 13.06 | 4 | 682.2544 |  |  |
| 137.492 | -2 4 7 | 24.47 | 4 | 2395.1236 |  |  |
| 137.922 | -4 2 10 | 65.45 | 4 | 17134.81 |  |  |
| 138.211 | -3 5 4 | 122.1 | 4 | 59633.64 |  |  |
| 138.541 | -6 4 1 | 5.63 | 4 | 126.7876 |  |  |
| 138.569 | -8 1 10 | 14.86 | 4 | 883.2784 |  |  |
| 138.593 | -1 5 4 | 4.48 | 4 | 80.2816 |  |  |
| 139.063 | -8 3 3 | 48.89 | 4 | 9560.9284 |  |  |
| 139.071 | 5 4 1 | 26.24 | 4 | 2754.1504 |  |  |
| 139.168 | -9 1 9 | 63.79 | 4 | 16276.6564 |  |  |
| 139.742 | 5 2 4 | 65.65 | 4 | 17239.69 |  |  |
| 139.983 | -8 3 7 | 201.09 | 4 | 161748.7524 | 140 | 19447971.66 |

1. **The calculation of**

Step 1: construct the hypothetical crystal, which has the same unit cell as that of the hessite. There is only one atom (Ag or Te) in the unit cell of the hypothetical crystal, and the only atom is located at the origin of the unit cell of the hypothetical crystal.

Step 2: generate all the possible reflection indices in the range of 0< 2θ ≤ 130º (Cu *K*α1) according to the unit cell parameters and space group of the hypothetical crystal. The space group of the hypothetical crystal in this case is *P*2/*m*, but just assuming the space group *P*1 for hypothetical crystals in any case does not change the structure of hypothetical crystals and will not lead to wrong results. In our calculations, the space group *P*1 is assumed for the hypothetical crystals.

Step 3: calculate *d* values for all the reflection indices generated in step 2 according to the unit cell parameters.

Step 4: calculate the atomic scattering factors of constitute elements (Ag and Te) for each *d* value obtained in step 3.

Step 5: sum up over all reflections in the desired 2θ to get .

Step 6: sum up over all atoms in the unit cell of the hessite to get .

The results of the calculations are given below. Note that the subscript in the following tables represents the index of only one reflection in a symmetrically equivalent group, and therefore the multiplicity is incorporated in the calculation of . In the main text of this paper, the subscript represents all possible reflection indices in a symmetrically equivalent group. Thus defined in the main text is equivalent to reported in the following table.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| 2θ |  |  | Multiplicity |  | 2θUL |  |
| 11.75 | -1 0 1 | 45.53 | 2 | 4145.9618 |  |  |
| 11.904 | 0 0 1 | 45.5 | 2 | 4140.5 |  |  |
| 13.095 | 1 0 0 | 45.21 | 2 | 4087.8882 |  |  |
| 19.766 | -1 0 2 | 43.36 | 2 | 3760.1792 |  |  |
| 19.855 | 0 1 0 | 43.33 | 2 | 3754.9778 |  |  |
| 21.937 | -2 0 1 | 42.69 | 2 | 3644.8722 |  |  |
| 22.191 | 1 0 1 | 42.61 | 2 | 3631.2242 |  |  |
| 23.132 | -1 -1 1 | 42.31 | 2 | 3580.2722 |  |  |
| 23.132 | -1 1 1 | 42.31 | 2 | 3580.2722 |  |  |
| 23.213 | 0 1 1 | 42.29 | 2 | 3576.8882 |  |  |
| 23.213 | 0 -1 1 | 42.29 | 2 | 3576.8882 |  |  |
| 23.625 | -2 0 2 | 42.16 | 2 | 3554.9312 |  |  |
| 23.858 | 1 -1 0 | 42.08 | 2 | 3541.4528 |  |  |
| 23.858 | 1 1 0 | 42.08 | 2 | 3541.4528 |  |  |
| 23.94 | 0 0 2 | 42.06 | 2 | 3538.0872 |  |  |
| 26.365 | 2 0 0 | 41.27 | 2 | 3406.4258 |  |  |
| 28.159 | -1 -1 2 | 40.69 | 2 | 3311.3522 |  |  |
| 28.159 | -1 1 2 | 40.69 | 2 | 3311.3522 |  |  |
| 29.756 | -2 -1 1 | 40.17 | 2 | 3227.2578 |  |  |
| 29.756 | -2 1 1 | 40.17 | 2 | 3227.2578 |  |  |
| 29.947 | 1 -1 1 | 40.1 | 2 | 3216.02 |  |  |
| 29.947 | 1 1 1 | 40.1 | 2 | 3216.02 | 30 | 78571.534 |
| 30.484 | -2 0 3 | 39.93 | 2 | 3188.8098 |  |  |
| 30.671 | -1 0 3 | 39.86 | 2 | 3177.6392 |  |  |
| 31.047 | -2 1 2 | 39.74 | 2 | 3158.5352 |  |  |
| 31.047 | -2 -1 2 | 39.74 | 2 | 3158.5352 |  |  |
| 31.293 | 0 -1 2 | 39.66 | 2 | 3145.8312 |  |  |
| 31.293 | 0 1 2 | 39.66 | 2 | 3145.8312 |  |  |
| 32.935 | -3 0 2 | 39.12 | 2 | 3060.7488 |  |  |
| 33.224 | 2 1 0 | 39.03 | 2 | 3046.6818 |  |  |
| 33.224 | 2 -1 0 | 39.03 | 2 | 3046.6818 |  |  |
| 33.399 | 1 0 2 | 38.97 | 2 | 3037.3218 |  |  |
| 34.499 | -3 0 1 | 38.61 | 2 | 2981.4642 |  |  |
| 34.779 | 2 0 1 | 38.52 | 2 | 2967.5808 |  |  |
| 35.765 | -3 0 3 | 38.2 | 2 | 2918.48 |  |  |
| 36.251 | 0 0 3 | 38.04 | 2 | 2894.0832 |  |  |
| 36.647 | -2 -1 3 | 37.91 | 2 | 2874.3362 |  |  |
| 36.647 | -2 1 3 | 37.91 | 2 | 2874.3362 |  |  |
| 36.807 | -1 1 3 | 37.86 | 2 | 2866.7592 |  |  |
| 36.807 | -1 -1 3 | 37.86 | 2 | 2866.7592 |  |  |
| 38.754 | -3 1 2 | 37.23 | 2 | 2772.1458 |  |  |
| 38.754 | -3 -1 2 | 37.23 | 2 | 2772.1458 |  |  |
| 39.158 | 1 1 2 | 37.1 | 2 | 2752.82 |  |  |
| 39.158 | 1 -1 2 | 37.1 | 2 | 2752.82 | 40 | 144031.8806 |
| 40.007 | 3 0 0 | 36.83 | 2 | 2712.8978 |  |  |
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| 86.713 | -4 0 8 | 25.96 | 2 | 1347.8432 |  |  |
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| 2θ |  |  | Multiplicity |  | 2θUL |  |
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| 11.904 | 0 0 1 | 50.09 | 2 | 5018.0162 |  |  |
| 13.095 | 1 0 0 | 49.73 | 2 | 4946.1458 |  |  |
| 19.766 | -1 0 2 | 47.43 | 2 | 4499.2098 |  |  |
| 19.855 | 0 1 0 | 47.4 | 2 | 4493.52 |  |  |
| 21.937 | -2 0 1 | 46.63 | 2 | 4348.7138 |  |  |
| 22.191 | 1 0 1 | 46.53 | 2 | 4330.0818 |  |  |
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| 30.484 | -2 0 3 | 43.48 | 2 | 3781.0208 |  |  |
| 30.671 | -1 0 3 | 43.42 | 2 | 3770.5928 |  |  |
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| 30 | 78571.534 | 93774.2178 | 1003669.143 | 350277.2376 | 2.865356453 |
| 40 | 144031.8806 | 171637.2802 | 1838804.166 | 1584255.518 | 1.160673985 |
| 50 | 275965.4414 | 331211.1756 | 3532568.234 | 3485458.526 | 1.013516072 |
| 60 | 387448.6172 | 469259.9974 | 4976628.927 | 4332256.612 | 1.148738261 |
| 70 | 533552.4896 | 654076.1426 | 6884724.487 | 6207733.484 | 1.109056068 |
| 80 | 689967.5864 | 854913.7372 | 8939395.64 | 9182239.436 | 0.973552879 |
| 90 | 837573.904 | 1045797.389 | 10883780.79 | 10836496.86 | 1.004363396 |
| 100 | 976400.4686 | 1225271.941 | 12712291.51 | 11786339.44 | 1.078561463 |
| 110 | 1131542.911 | 1424945.849 | 14752126.68 | 14095343.51 | 1.046595755 |
| 120 | 1251082.155 | 1577507.146 | 16318685.82 | 16333185.08 | 0.999112282 |
| 130 | 1367290.901 | 1724781.397 | 17837452.8 | 17850981.39 | 0.999242137 |
| 140 | 1474678.201 | 1859797.567 | 19236615.88 | 19447971.66 | 0.989132245 |