Table 6,1,1,4, Coefficients for analytical approximation to the scattering factors of Tables 6,1,1,1 and 6,1,13

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | a1 | b1 | a2 | b2 | a3 | b3 | a4 | b4 | c | Maximum  error | sin в/Х  (A -1) | Mean  error |
| H | SDS | 0,493002 | 10,5109 | 0,322912 | 26,1257 | 0,140191 | 3,14236 | 0,040810 | 57,7997 | 0,003038 | 0,000 | 0,00 | 0,000 |
| H | HF | 0,489918 20,6593 | | 0,262003 | 7,74039 | 0,196767 | 49,5519 | 0,049879 | 2,20159 | 0,001305 | 0,000 | 0,17 | 0,000 |
| h1- | HF | 0,897661 | 53,1368 | 0,565616 | 15,1870 | 0,415815 | 186,576 | 0,116973 | 3,56709 | 0,002389 | 0,002 | 0,09 | 0,001 |
| He | RHF | 0,873400 | 9,10370 | 0,630900 | 3,35680 | 0,311200 | 22,9276 | 0,178000 | 0,982100 | 0,006400 | 0,001 | 1,01 | 0,000 |
| Li | RHF | 1,12820 | 3,95460 | 0,750800 | 1,05240 | 0,617500 | 85,3905 | 0,465300 | 168,261 | 0,037700 | 0,005 | 2,00 | 0,001 |
| Li1+ | RHF | 0,696800 | 4,62370 | 0,788800 | 1,95570 | 0,341400 | 0,631600 | 0,156300 | 10,0953 | 0,016700 | 0,001 | 1,78 | 0,000 |
| Be | RHF | 1,59190 | 43,6427 | 1,12780 | 1,86230 | 0,539100 | 103,483 | 0,702900 | 0,542000 | 0,038500 | 0,003 | 0,56 | 0,001 |
| Be2+ | RHF | 6,26030 | 0,002700 | 0,884900 | 0,831300 | 0,799300 | 2,27580 | 0,164700 | 5,11460 | - 6,1092 | 0,001 | 1,97 | 0,000 |
| B | RHF | 2,05450 | 23,2185 | 1,33260 | 1,02100 | 1,09790 | 60,3498 | 0,706800 | 0,140300 | -0,19320 | 0,002 | 0,75 | 0,001 |
| C | RHF | 2,31000 | 20,8439 | 1,02000 | 10,2075 | 1,58860 | 0,568700 | 0,865000 | 51,6512 | 0,215600 | 0,006 | 2,00 | 0,001 |
| C | HF | 2,26069 | 22,6907 | 1,56165 | 0,656665 | 1,05075 | 9,75618 | 0,839259 | 55,5949 | 0,286977 | 0,001 | 0,16 | 0,000 |
| N | RHF | 12,2126 | 0,005700 | 3,13220 | 9,89330 | 2,01250 | 28,9975 | 1,16630 | 0,582600 | -11,529 | 0,007 | 0,11 | 0,002 |
| O | RHF | 3,04850 | 13,2771 | 2,28680 | 5,70110 | 1,54630 | 0,323900 | 0,867000 | 32,9089 | 0,250800 | 0,001 | 0,22 | 0,000 |
| O1- | HF | 4,19160 | 12,8573 | 1,63969 | 4,17236 | 1,52673 | 47,0179 | -20,307 | - 0,01404 | 21,9412 | 0,011 | 1,50 | 0,004 |
| F | RHF | 3,53920 | 10,2825 | 2,64120 | 4,29440 | 1,51700 | 0,261500 | 1,02430 | 26,1476 | 0,277600 | 0,001 | 0,01 | 0,000 |
| F1- | HF | 3,63220 | 5,27756 | 3,51057 | 14,7353 | 1,26064 | 0,442258 | 0,940706 | 47,3437 | 0,653396 | 0,003 | 0,09 | 0,001 |
| Ne | RHF | 3,95530 | 8,40420 | 3,11250 | 3,42620 | 1,45460 | 0,230600 | 1,12510 | 21,7184 | 0,351500 | 0,002 | 0,25 | 0,001 |
| Na | RHF | 4,76260 | 3,28500 | 3,17360 | 8,84220 | 1,26740 | 0,313600 | 1,11280 | 129,424 | 0,676000 | 0,009 | 0,13 | 0,002 |
| Na1+ | RHF | 3,25650 | 2,66710 | 3,93620 | 6,11530 | 1,39980 | 0,200100 | 1,00320 | 14,0390 | 0,404000 | 0,001 | 0,70 | 0,000 |
| Mg | RHF | 5,42040 | 2,82750 | 2,17350 | 79,2611 | 1,22690 | 0,380800 | 2,30730 | 7,19370 | 0,858400 | 0,015 | 0,08 | 0,003 |
| Mg2+ | RHF | 3,49880 | 2,16760 | 3,83780 | 4,75420 | 1,32840 | 0,185000 | 0,849700 | 10,1411 | 0,485300 | 0,001 | 1,34 | 0,000 |
| Al | RHF | 6,42020 | 3,03870 | 1,90020 | 0,742600 | 1,59360 | 31,5472 | 1,96460 | 85,0886 | 1,11510 | 0,018 | 2,00 | 0,005 |
| Al3+ | HF | 4,17448 | 1,93816 | 3,38760 | 4,14553 | 1,20296 | 0,228753 | 0,528137 | 8,28524 | 0,706786 | 0,000 | 1,50 | 0,000 |
| Siv | RHF | 6,29150 | 2,43860 | 3,03530 | 32,3337 | 1,98910 | 0,678500 | 1,54100 | 81,6937 | 1,14070 | 0,009 | 2,00 | 0,002 |
| Sival | HF | 5,66269 | 2,66520 | 3,07164 | 38,6634 | 2,62446 | 0,916946 | 1,39320 | 93,5458 | 1,24707 | 0,001 | 0,53 | 0,001 |
| Si4+ | HF | 4,43918 | 1,64167 | 3,20345 | 3,43757 | 1,19453 | 0,214900 | 0,416530 | 6,65365 | 0,746297 | 0,000 | 1,50 | 0,000 |
| P | RHF | 6,43450 | 1,90670 | 4,17910 | 27,1570 | 1,78000 | 0,526000 | 1,49080 | 68,1645 | 1,11490 | 0,003 | 0,65 | 0,001 |
| S | RHF | 6,90530 | 1,46790 | 5,20340 | 22,2151 | 1,43790 | 0,253600 | 1,58630 | 56,1720 | 0,866900 | 0,005 | 0,67 | 0,002 |
| Cl | RHF | 11,4604 | 0,010400 | 7,19640 | 1,16620 | 6,25560 | 18,5194 | 1,64550 | 47,7784 | -9,5574 | 0,007 | 0,78 | 0,003 |
| Cl1- | RHF | 18,2915 | 0,006600 | 7,20840 | 1,17170 | 6,53370 | 19,5424 | 2,33860 | 60,4486 | -16,378 | 0,007 | 0,76 | 0,003 |
| Ar | RHF | 7,48450 | 0,907200 | 6,77230 | 14,8407 | 0,653900 | 43,8983 | 1,64420 | 33,3929 | 1,44450 | 0,029 | 2,00 | 0,006 |
| К | RHF | 8,21860 | 12,7949 | 7,43980 | 0,774800 | 1,05190 | 213,187 | 0,865900 | 41,6841 | 1,42280 | 0,011 | 0,90 | 0,005 |
| K1+ | RHF | 7,95780 | 12,6331 | 7,49170 | 0,767400 | 6,35900 | -0,00200 | 1,19150 | 31,9128 | - 4,9978 | 0,011 | 0,91 | 0,005 |
| Ca | RHF | 8,62660 | 10,4421 | 7,38730 | 0,659900 | 1,58990 | 85,7484 | 1,02110 | 178,437 | 1,37510 | 0,016 | 0,99 | 0,006 |
| Ca2+ | RHF | 15,6348 | -0,00740 | 7,95180 | 0,608900 | 8,43720 | 10,3116 | 0,853700 | 25,9905 | -14,875 | 0,017 | 2,00 | 0,004 |
| Sc | RHF | 9,18900 | 9,02130 | 7,36790 | 0,572900 | 1,64090 | 136,108 | 1,46800 | 51,3531 | 1,33290 | 0,014 | 1,07 | 0,006 |
| Sc3+ | HF | 13,4008 | 0,298540 | 8,02730 | 7,96290 | 1,65943 | -0,28604 | 1,57936 | 16,0662 | - 6,6667 | 0,002 | 1,50 | 0,000 |
| Ti | RHF | 9,75950 | 7,85080 | 7,35580 | 0,500000 | 1,69910 | 35,6338 | 1,90210 | 116,105 | 1,28070 | 0,014 | 2,00 | 0,006 |
| Ti2+ | HF | 9,11423 | 7,52430 | 7,62174 | 0,457585 | 2,27930 | 19,5361 | 0,087899 | 61,6558 | 0,897155 | 0,006 | 1,50 | 0,001 |
| Ti3+ | HF | 17,7344 | 0,220610 | 8,73816 | 7,04716 | 5,25691 | -0,15762 | 1,92134 | 15,9768 | -14,652 | 0,001 | 0,00 | 0,000 |
| Ti4+ | HF | 19,5114 | 0,178847 | 8,23473 | 6,67018 | 2,01341 | -0,29263 | 1,52080 | 12,9464 | -13,280 | 0,002 | 1,50 | 0,000 |
| V | RHF | 10,2971 | 6,86570 | 7,35110 | 0,438500 | 2,07030 | 26,8938 | 2,05710 | 102,478 | 1,21990 | 0,014 | 2,00 | 0,005 |
| v2+ | RHF | 10,1060 | 6,88180 | 7,35410 | 0,440900 | 2,28840 | 20,3004 | 0,022300 | 115,122 | 1,22980 | 0,015 | 2,00 | 0,004 |
| v3+ | HF | 9,43141 | 6,39535 | 7,74190 | 0,383349 | 2,15343 | 15,1908 | 0,016865 | 63,9690 | 0,656565 | 0,004 | 1,50 | 0,001 |
| v5+ | HF | 15,6887 | 0,679003 | 8,14208 | 5,40135 | 2,03081 | 9,97278 | -9,5760 | 0,940464 | 1,71430 | 0,000 | 0,34 | 0,000 |
| Cr | RHF | 10,6406 | 6,10380 | 7,35370 | 0,392000 | 3,32400 | 20,2626 | 1,49220 | 98,7399 | 1,18320 | 0,011 | 2,00 | 0,004 |
| Cr2+ | HF | 9,54034 | 5,66078 | 7,75090 | 0,344261 | 3,58274 | 13,3075 | 0,509107 | 32,4224 | 0,616898 | 0,002 | 1,50 | 0,000 |
| Cr3+ | HF | 9,68090 | 5,59463 | 7,81136 | 0,334393 | 2,87603 | 12,8288 | 0,113575 | 32,8761 | 0,518275 | 0,002 | 1,50 | 0,000 |
| Mn | RHF | 11,2819 | 5,34090 | 7,35730 | 0,343200 | 3,01930 | 17,8674 | 2,24410 | 83,7543 | 1,08960 | 0,009 | 2,00 | 0,004 |
| Mn2+ | RHF | 10,8061 | 5,27960 | 7,36200 | 0,343500 | 3,52680 | 14,3430 | 0,218400 | 41,3235 | 1,08740 | 0,009 | 2,00 | 0,002 |
| Mn3+ | HF | 9,84521 | 4,91797 | 7,87194 | 0,294393 | 3,56531 | 10,8171 | 0,323613 | 24,1281 | 0,393974 | 0,001 | 1,50 | 0,000 |
| Mn4+ | HF | 9,96253 | 4,84850 | 7,97057 | 0,283303 | 2,76067 | 10,4852 | 0,054447 | 27,5730 | 0,251877 | 0,001 | 1,50 | 0,000 |
| Fe | RHF | 11,7695 | 4,76110 | 7,35730 | 0,307200 | 3,52220 | 15,3535 | 2,30450 | 76,8805 | 1,03690 | 0,011 | 0,08 | 0,004 |
| Fe2+ | RHF | 11,0424 | 4,65380 | 7,37400 | 0,305300 | 4,13460 | 12,0546 | 0,439900 | 31,2809 | 1,00970 | 0,008 | 2,00 | 0,002 |
| Fe3+ | RHF | 11,1764 | 4,61470 | 7,38630 | 0,300500 | 3,39480 | 11,6729 | 0,072400 | 38,5566 | 0,970700 | 0,008 | 2,00 | 0,002 |
| Co | RHF | 12,2841 | 4,27910 | 7,34090 | 0,278400 | 4,00340 | 13,5359 | 2,34880 | 71,1692 | 1,01180 | 0,013 | 0,08 | 0,004 |
| Co2+ | RHF | 11,2296 | 4,12310 | 7,38830 | 0,272600 | 4,73930 | 10,2443 | 0,710800 | 25,6466 | 0,932400 | 0,006 | 2,00 | 0,001 |
| Co3+ | HF | 10,3380 | 3,90969 | 7,88173 | 0,238668 | 4,76795 | 8,35583 | 0,725591 | 18,3491 | 0,286667 | 0,000 | 1,50 | 0,000 |
| Ni | RHF | 12,8376 | 3,87850 | 7,29200 | 0,256500 | 4,44380 | 12,1763 | 2,38000 | 66,3421 | 1,0341 | 0,014 | 0,08 | 0,004 |
| Ni2+ | RHF | 11,4166 | 3,67660 | 7,40050 | 0,244900 | 5,34420 | 8,87300 | 0,977300 | 22,1626 | 0,861400 | 0,003 | 2,00 | 0,001 |
| Ni3+ | HF | 10,7806 | 3,54770 | 7,75868 | 0,223140 | 5,22746 | 7,64468 | 0,847114 | 16,9673 | 0,386044 | 0,000 | 0,57 | 0,000 |
| Cu | RHF | 13,3380 | 3,58280 | 7,16760 | 0,247000 | 5,61580 | 11,3966 | 1,67350 | 64,8126 | 1,19100 | 0,015 | 0,08 | 0,005 |
| Cu1+ | RHF | 11,9475 | 3,36690 | 7,35730 | 0,227400 | 6,24550 | 8,66250 | 1,55780 | 25,8487 | 0,89000 | 0,003 | 0,24 | 0,001 |
| Cu2+ | HF | 11,8168 | 3,37484 | 7,11181 | 0,244078 | 5,78135 | 7,98760 | 1,14523 | 19,8970 | 1,14431 | 0,001 | 0,26 | 0,000 |
| Zn | RHF | 14,0743 | 3,26550 | 7,03180 | 0,233300 | 5,16520 | 10,3163 | 2,41000 | 58,7097 | 1,30410 | 0,016 | 0,08 | 0,005 |
| Zn2+ | RHF | 11,9719 | 2,99460 | 7,38620 | 0,203100 | 6,46680 | 7,08260 | 1,39400 | 18,0995 | 0,780700 | 0,001 | 0,62 | 0,000 |
| Ga | RHF | 15,2354 | 3,06690 | 6,70060 | 0,241200 | 4,35910 | 10,7805 | 2,96230 | 61,4135 | 1,71890 | 0,025 | 0,08 | 0,008 |
| Ga3+ | HF | 12,6920 | 2,81262 | 6,69883 | 0,227890 | 6,06692 | 6,36441 | 1,00660 | 14,4122 | 1,53545 | 0,008 | 1,45 | 0,000 |
| Ge | RHF | 16,0816 | 2,85090 | 6,37470 | 0,251600 | 3,70680 | 11,4468 | 3,68300 | 54,7625 | 2,13130 | 0,024 | 0,08 | 0,008 |
| Ge4+ | HF | 12,9172 | 2,53718 | 6,70003 | 0,205855 | 6,06791 | 5,47913 | 0,859041 | 11,6030 | 1,45572 | 0,000 | 0,32 | 0,000 |

Table 6,1,1,4, Coefficients for analytical approximation to scattering factors (cont,)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | a1 | N | a2 | b2 | a3 | Ь3 | a4 | Ь4 | c | Maximum  error | sin в/Х  (A -1) | Mean  error |
| As | RHF | 16,6723 | 2,63450 | 6,07010 | 0,264700 | 3,43130 | 12,9479 | 4,27790 | 47,7972 | 2,53100 | 0,019 | 0,09 | 0,008 |
| Se | RHF | 17,0006 | 2,40980 | 5,81960 | 0,272600 | 3,97310 | 15,2372 | 4,35430 | 43,8163 | 2,84090 | 0,016 | 2,00 | 0,006 |
| Br | RHF | 17,1789 | 2,17230 | 5,23580 | 16,5796 | 5,63770 | 0,260900 | 3,98510 | 41,4328 | 2,95570 | 0,012 | 2,00 | 0,004 |
| Br1- | RHF | 17,1718 | 2,20590 | 6,33380 | 19,3345 | 5,57540 | 0,287100 | 3,72720 | 58,1535 | 3,17760 | 0,016 | 2,00 | 0,006 |
| Kr | RHF | 17,3555 | 1,93840 | 6,72860 | 16,5623 | 5,54930 | 0,226100 | 3,53750 | 39,3972 | 2,82500 | 0,008 | 2,00 | 0,002 |
| Rb | RHF | 17,1784 | 1,78880 | 9,64350 | 17,3151 | 5,13990 | 0,274800 | 1,52920 | 164,934 | 3,48730 | 0,028 | 0,12 | 0,008 |
| Rb1+ | RHF | 17,5816 | 1,71390 | 7,65980 | 14,7957 | 5,89810 | 0,160300 | 2,78170 | 31,2087 | 2,07820 | 0,002 | 1,99 | 0,001 |
| Sr | RHF | 17,5663 | 1,55640 | 9,81840 | 14,0988 | 5,42200 | 0,166400 | 2,66940 | 132,376 | 2,50640 | 0,021 | 0,13 | 0,005 |
| Sr2+ | RHF | 18,0874 | 1,49070 | 8,13730 | 12,6963 | 2,56540 | 24,5651 | -34,193 | -0,01380 | 41,4025 | 0,008 | 2,00 | 0,002 |
| Y | \*RHF | 17,7760 | 1,40290 | 10,2946 | 12,8006 | 5,72629 | 0,125599 | 3,26588 | 104,354 | 1,91213 | 0,028 | 0,07 | 0,006 |
| Y3+ | \*DS | 17,9268 | 1,35417 | 9,15310 | 11,2145 | 1,76795 | 22,6599 | -33,108 | -0,01319 | 40,2602 | 0,005 | 2,00 | 0,001 |
| Zr | \*RHF | 17,8765 | 1,27618 | 10,9480 | 11,9160 | 5,41732 | 0,117622 | 3,65721 | 87,6627 | 2,06929 | 0,035 | 0,07 | 0,008 |
| Zr4+ | \*DS | 18,1668 | 1,21480 | 10,0562 | 10,1483 | 1,01118 | 21,6054 | -2,6479 | -0,10276 | 9,41454 | 0,004 | 2,00 | 0,001 |
| Nb | \*RHF | 17,6142 | 1,18865 | 12,0144 | 11,7660 | 4,04183 | 0,204785 | 3,53346 | 69,7957 | 3,75591 | 0,042 | 0,08 | 0,011 |
| Nb3+ | \*DS | 19,8812 | 0,019175 | 18,0653 | 1,13305 | 11,0177 | 10,1621 | 1,94715 | 28,3389 | -12,912 | 0,006 | 2,00 | 0,002 |
| Nb5+ | \*DS | 17,9163 | 1,12446 | 13,3417 | 0,028781 | 10,7990 | 9,28206 | 0,337905 | 25,7228 | -6,3934 | 0,007 | 2,00 | 0,003 |
| Mo | RHF | 3,70250 | 0,277200 | 17,2356 | 1,09580 | 12,8876 | 11,0040 | 3,74290 | 61,6584 | 4,38750 | 0,046 | 0,08 | 0,012 |
| Mo3+ | \*DS | 21,1664 | 0,014734 | 18,2017 | 1,03031 | 11,7423 | 9,53659 | 2,30951 | 26,6307 | -14,421 | 0,009 | 2,00 | 0,003 |
| Mo5+ | \*DS | 21,0149 | 0,014345 | 18,0992 | 1,02238 | 11,4632 | 8,78809 | 0,740625 | 23,3452 | -14,316 | 0,010 | 2,00 | 0,003 |
| Mo6+ | \*DS | 17,8871 | 1,03649 | 11,1750 | 8,48061 | 6,57891 | 0,058881 | 0,000000 | 0,000000 | 0,344941 | 0,014 | 0,00 | 0,006 |
| Tc | \*RHF | 19,1301 | 0,864132 | 11,0948 | 8,14487 | 4,64901 | 21,5707 | 2,71263 | 86,8472 | 5,40428 | 0,061 | 2,00 | 0,011 |
| Ru | \*RHF | 19,2674 | 0,808520 | 12,9182 | 8,43467 | 4,86337 | 24,7997 | 1,56756 | 94,2928 | 5,37874 | 0,041 | 2,00 | 0,006 |
| Ru3+ | \*DS | 18,5638 | 0,847329 | 13,2885 | 8,37164 | 9,32602 | 0,017662 | 3,00964 | 22,8870 | -3,1892 | 0,013 | 2,00 | 0,004 |
| Ru4+ | \*DS | 18,5003 | 0,844582 | 13,1787 | 8,12534 | 4,71304 | 0,36495 | 2,18535 | 20,8504 | 1,42357 | 0,014 | 2,00 | 0,004 |
| Rh | \*RHF | 19,2957 | 0,751536 | 14,3501 | 8,21758 | 4,73425 | 25,8749 | 1,28918 | 98,6062 | 5,32800 | 0,021 | 2,00 | 0,004 |
| Rh3+ | \*DS | 18,8785 | 0,764252 | 14,1259 | 7,84438 | 3,32515 | 21,2487 | -6,1989 | -0,01036 | 11,8678 | 0,014 | 2,00 | 0,004 |
| Rh4+ | \*DS | 18,8545 | 0,760825 | 13,9806 | 7,62436 | 2,53464 | 19,3317 | -5,6526 | -0,01020 | 11,2835 | 0,014 | 2,00 | 0,003 |
| Pd | \*RHF | 19,3319 | 0,698655 | 15,5017 | 7,98929 | 5,29537 | 25,2052 | 0,605844 | 76,8986 | 5,26593 | 0,012 | 1,08 | 0,005 |
| Pd2+ | \*DS | 19,1701 | 0,696219 | 15,2096 | 7,55573 | 4,32234 | 22,5057 | 0,000000 | 0,000000 | 5,29160 | 0,011 | 2,00 | 0,004 |
| Pd4+ | \*DS | 19,2493 | 0,683839 | 14,7900 | 7,14833 | 2,89289 | 17,9144 | -7,9492 | 0,005127 | 13,0174 | 0,014 | 2,00 | 0,003 |
| Ag | RHF | 19,2808 | 0,644600 | 16,6885 | 7,47260 | 4,80450 | 24,6605 | 1,04630 | 99,8156 | 5,17900 | 0,016 | 1,14 | 0,007 |
| Ag1+ | \*DS | 19,1812 | 0,646179 | 15,9719 | 7,19123 | 5,27475 | 21,7326 | 0,357534 | 66,1147 | 5,21572 | 0,012 | 1,13 | 0,005 |
| Ag2+ | \*DS | 19,1643 | 0,645643 | 16,2456 | 7,18544 | 4,37090 | 21,4072 | 0,000000 | 0,000000 | 5,21404 | 0,011 | 1,14 | 0,005 |
| Cd | RHF | 19,2214 | 0,594600 | 17,6444 | 6,90890 | 4,46100 | 24,7008 | 1,60290 | 87,4825 | 5,06940 | 0,020 | 2,00 | 0,008 |
| Cd2+ | \*DS | 19,1514 | 0,597922 | 17,2535 | 6,80639 | 4,47128 | 20,2521 | 0,000000 | 0,000000 | 5,11937 | 0,014 | 1,17 | 0,007 |
| In | RHF | 19,1624 | 0,547600 | 18,5596 | 6,37760 | 4,29480 | 25,8499 | 2,03960 | 92,8029 | 4,93910 | 0,027 | 2,00 | 0,009 |
| In3+ | \*DS | 19,1045 | 0,551522 | 18,1108 | 6,32470 | 3,78897 | 17,3595 | 0,000000 | 0,000000 | 4,99635 | 0,022 | 2,00 | 0,007 |
| Sn | RHF | 19,1889 | 5,83030 | 19,1005 | 0,503100 | 4,45850 | 26,8909 | 2,46630 | 83,9571 | 4,78210 | 0,032 | 2,00 | 0,009 |
| Sn2+ | RHF | 19,1094 | 0,503600 | 19,0548 | 5,83780 | 4,56480 | 23,3752 | 0,487000 | 62,2061 | 4,78610 | 0,032 | 2,00 | 0,009 |
| Sn4+ | RHF | 18,9333 | 5,76400 | 19,7131 | 0,465500 | 3,41820 | 14,0049 | 0,019300 | -0,75830 | 3,91820 | 0,016 | 2,00 | 0,004 |
| Sb | RHF | 19,6418 | 5,30340 | 19,0455 | 0,460700 | 5,03710 | 27,9074 | 2,68270 | 75,2825 | 4,59090 | 0,035 | 2,00 | 0,009 |
| Sb3+ | \*DS | 18,9755 | 0,467196 | 18,9330 | 5,22126 | 5,10789 | 19,5902 | 0,288753 | 55,5113 | 4,69626 | 0,028 | 2,00 | 0,007 |
| Sb5+ | \*DS | 19,8685 | 5,44853 | 19,0302 | 0,467973 | 2,41253 | 14,1259 | 0,000000 | 0,000000 | 4,69263 | 0,030 | 2,00 | 0,008 |
| Te | \*RHF | 19,9644 | 4,81742 | 19,0138 | 0,420885 | 6,14487 | 28,5284 | 2,52390 | 70,8403 | 4,35200 | 0,038 | 2,00 | 0,009 |
| I | RHF | 20,1472 | 4,34700 | 18,9949 | 0,381400 | 7,51380 | 27,7660 | 2,27350 | 66,8776 | 4,07120 | 0,037 | 2,00 | 0,009 |
| I1- | RHF | 20,2332 | 4,35790 | 18,9970 | 0,381500 | 7,80690 | 29,5259 | 2,88680 | 84,9304 | 4,07140 | 0,038 | 2,00 | 0,009 |
| Xe | RHF | 20,2933 | 3,92820 | 19,0298 | 0,344000 | 8,97670 | 26,4659 | 1,99000 | 64,2658 | 3,71180 | 0,038 | 2,00 | 0,009 |
| Cs | RHF | 20,3892 | 3,56900 | 19,1062 | 0,310700 | 10,6620 | 24,3879 | 1,49530 | 213,904 | 3,33520 | 0,032 | 2,00 | 0,010 |
| Cs1+ | RHF | 20,3524 | 3,55200 | 19,1278 | 0,308600 | 10,2821 | 23,7128 | 0,961500 | 59,4565 | 3,27910 | 0,037 | 2,00 | 0,009 |
| Ba | RHF | 20,3361 | 3,21600 | 19,2970 | 0,275600 | 10,8880 | 20,2073 | 2,69590 | 167,202 | 2,77310 | 0,032 | 2,00 | 0,009 |
| Ba2+ | \*DS | 20,1807 | 3,21367 | 19,1136 | 0,283310 | 10,9054 | 20,0558 | 0,77634 | 51,7460 | 3,02902 | 0,029 | 2,00 | 0,007 |
| La | \*RHF | 20,5780 | 2,94817 | 19,5990 | 0,244475 | 11,3727 | 18,7726 | 3,28719 | 133,124 | 2,14678 | 0,032 | 2,00 | 0,009 |
| La3+ | \*DS | 20,2489 | 2,92070 | 19,3763 | 0,250698 | 11,6323 | 17,8211 | 0,336048 | 54,9453 | 2,40860 | 0,028 | 2,00 | 0,007 |
| Ce | \*RHF | 21,1671 | 2,81219 | 19,7695 | 0,226836 | 11,8513 | 17,6083 | 3,33049 | 127,113 | 1,86264 | 0,026 | 2,00 | 0,008 |
| Ce3+ | \*DS | 20,8036 | 2,77691 | 19,5590 | 0,231540 | 11,9369 | 16,5408 | 0,612376 | 43,1692 | 2,09013 | 0,023 | 2,00 | 0,005 |
| Ce4+ | \*DS | 20,3235 | 2,65941 | 19,8186 | 0,218850 | 12,1233 | 15,7992 | 0,144583 | 62,2355 | 1,59180 | 0,026 | 2,00 | 0,007 |
| Pr | \*RHF | 22,0440 | 2,77393 | 19,6697 | 0,222087 | 12,3856 | 16,7669 | 2,82428 | 143,644 | 2,05830 | 0,021 | 0,12 | 0,007 |
| Pr3+ | \*DS | 21,3727 | 2,64520 | 19,7491 | 0,214299 | 12,1329 | 15,3230 | 0,975180 | 36,4065 | 1,77132 | 0,019 | 2,00 | 0,004 |
| Pr4+ | \*DS | 20,9413 | 2,54467 | 20,0539 | 0,202481 | 12,4668 | 14,8137 | 0,296689 | 45,4643 | 1,24285 | 0,021 | 2,00 | 0,005 |
| Nd | \*RHF | 22,6845 | 2,66248 | 19,6847 | 0,210628 | 12,7740 | 15,8850 | 2,85137 | 137,903 | 1,98486 | 0,024 | 0,13 | 0,007 |
| Nd3+ | \*DS | 21,9610 | 2,52722 | 19,9339 | 0,199237 | 12,1200 | 14,1783 | 1,51031 | 30,8717 | 1,47588 | 0,015 | 2,00 | 0,003 |
| Pm | \*RHF | 23,3405 | 2,56270 | 19,6095 | 0,202088 | 13,1235 | 15,1009 | 2,87516 | 132,721 | 2,02876 | 0,026 | 0,13 | 0,008 |
| Pm3+ | \*DS | 22,5527 | 2,41740 | 20,1108 | 0,185769 | 12,0671 | 13,1275 | 2,07492 | 27,4491 | 1,19499 | 0,012 | 2,00 | 0,002 |
| Sm | \*RHF | 24,0042 | 2,47274 | 19,4258 | 0,196451 | 13,4396 | 14,3996 | 2,89604 | 128,007 | 2,20963 | 0,029 | 0,13 | 0,009 |
| Sm3+ | \*DS | 23,1504 | 2,31641 | 20,2599 | 0,174081 | 11,9202 | 12,1571 | 2,71488 | 24,8242 | 0,954586 | 0,009 | 2,00 | 0,002 |
| Eu | RHF | 24,6274 | 2,38790 | 19,0886 | 0,194200 | 13,7603 | 13,7546 | 2,92270 | 123,174 | 2,57450 | 0,031 | 0,14 | 0,010 |
| Eu2+ | \*DS | 24,0063 | 2,27783 | 19,9504 | 0,173530 | 11,8034 | 11,6096 | 3,87243 | 26,5156 | 1,36389 | 0,004 | 2,00 | 0,002 |
| Eu3+ | \*DS | 23,7497 | 2,22258 | 20,3745 | 0,163940 | 11,8509 | 11,3110 | 3,26503 | 22,9966 | 0,759344 | 0,006 | 2,00 | 0,001 |
| Gd | \*RHF | 25,0709 | 2,25341 | 19,0798 | 0,181951 | 13,8518 | 12,9331 | 3,54545 | 101,398 | 2,41960 | 0,036 | 0,15 | 0,011 |
| Gd3+ | \*DS | 24,3466 | 2,13553 | 20,4208 | 0,155525 | 11,8708 | 10,5782 | 3,71490 | 21,7029 | 0,645089 | 0,004 | 2,00 | 0,001 |

Table 6,1,1,4, Coefficients for analytical approximation to scattering factors (cont,)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | ai | N | a2 | b2 | a3 | Ь3 | a4 | Ь4 | c | Maximum  error | sin в/Х  (A -1) | Mean  error |
| Tb | \*RHF | 25,8976 | 2,24256 | 18,2185 | 0,196143 | 14,3167 | 12,6648 | 2,95354 | 115,362 | 3,58324 | 0,035 | 0,14 | 0,012 |
| Tb3+ | \*DS | 24,9559 | 2,05601 | 20,3271 | 0,149525 | 12,2471 | 10,0499 | 3,77300 | 21,2773 | 0,691967 | 0,005 | 0,00 | 0,001 |
| Dy | \*RHF | 26,5070 | 2,18020 | 17,6383 | 0,202172 | 14,5596 | 12,1899 | 2,96577 | 111,874 | 4,29728 | 0,037 | 0,15 | 0,013 |
| Dy3+ | \*DS | 25,5395 | 1,98040 | 20,2861 | 0,143384 | 11,9812 | 9,34972 | 4,50073 | 19,5810 | 0,689690 | 0,003 | 0,00 | 0,001 |
| Ho | \*RHF | 26,9049 | 2,07051 | 17,2940 | 0,197940 | 14,5583 | 11,4407 | 3,63837 | 92,6566 | 4,56796 | 0,040 | 0,15 | 0,013 |
| Ho3+ | \*DS | 26,1296 | 1,91072 | 20,0994 | 0,139358 | 11,9788 | 8,80018 | 4,93676 | 18,5908 | 0,852795 | 0,003 | 0,00 | 0,001 |
| Er | \*RHF | 27,6563 | 2,07356 | 16,4285 | 0,223545 | 14,9779 | 11,3604 | 2,98233 | 105,703 | 5,92046 | 0,040 | 0,15 | 0,015 |
| Er3+ | \*DS | 26,7220 | 1,84659 | 19,7748 | 0,137290 | 12,1506 | 8,36225 | 5,17379 | 17,8974 | 1,17613 | 0,003 | 0,00 | 0,001 |
| Tm | \*RHF | 28,1819 | 2,02859 | 15,8851 | 0,238849 | 15,1542 | 10,9975 | 2,98706 | 102,961 | 6,75621 | 0,041 | 0,15 | 0,016 |
| Tm3+ | \*DS | 27,3083 | 1,78711 | 19,3320 | 0,136974 | 12,3339 | 7,96778 | 5,38348 | 17,2922 | 1,63929 | 0,003 | 0,00 | 0,001 |
| Yb | \*RHF | 28,6641 | 1,98890 | 15,4345 | 0,257119 | 15,3087 | 10,6647 | 2,98963 | 100,417 | 7,56672 | 0,042 | 0,15 | 0,016 |
| Yb2+ | \*DS | 28,1209 | 1,78503 | 17,6817 | 0,159970 | 13,3335 | 8,18304 | 5,14657 | 20,3900 | 3,70983 | 0,008 | 0,00 | 0,003 |
| Yb3+ | \*DS | 27,8917 | 1,73272 | 18,7614 | 0,138790 | 12,6072 | 7,64412 | 5,47647 | 16,8153 | 2,26001 | 0,003 | 0,00 | 0,002 |
| Lu | \*RHF | 28,9476 | 1,90182 | 15,2208 | 9,98519 | 15,1000 | 0,261033 | 3,71601 | 84,3298 | 7,97628 | 0,043 | 0,16 | 0,016 |
| Lu3+ | \*DS | 28,4628 | 1,68216 | 18,1210 | 0,142292 | 12,8429 | 7,33727 | 5,59415 | 16,3535 | 2,97573 | 0,004 | 0,14 | 0,002 |
| Hf | \*RHF | 29,1440 | 1,83262 | 15,1726 | 9,59990 | 14,7586 | 0,275116 | 4,30013 | 72,0290 | 8,58154 | 0,047 | 0,08 | 0,016 |
| Hf4+ | \*DS | 28,8131 | 1,59136 | 18,4601 | 0,128903 | 12,7285 | 6,76232 | 5,59927 | 14,0366 | 2,39699 | 0,002 | 0,00 | 0,001 |
| Ta | \*RHF | 29,2024 | 1,77333 | 15,2293 | 9,37046 | 14,5135 | 0,295977 | 4,76492 | 63,3644 | 9,24354 | 0,049 | 0,08 | 0,017 |
| Ta5+ | \*DS | 29,1587 | 1,50711 | 18,8407 | 0,116741 | 12,8268 | 6,31524 | 5,38695 | 12,4244 | 1,78555 | 0,002 | 2,00 | 0,001 |
| W | \*RHF | 29,0818 | 1,72029 | 15,4300 | 9,22590 | 14,4327 | 0,321703 | 5,11982 | 57,0560 | 9,88750 | 0,051 | 0,09 | 0,017 |
| w6+ | \*DS | 29,4936 | 1,42755 | 19,3763 | 0,104621 | 13,0544 | 5,93667 | 5,06412 | 11,1972 | 1,01074 | 0,001 | 0,00 | 0,000 |
| Re | \*RHF | 28,7621 | 1,67191 | 15,7189 | 9,09227 | 14,5564 | 0,350500 | 5,44174 | 52,0861 | 10,4720 | 0,052 | 0,09 | 0,017 |
| Os | \*RHF | 28,1894 | 1,62903 | 16,1550 | 8,97948 | 14,9305 | 0,382661 | 5,67589 | 48,1647 | 11,0005 | 0,051 | 0,09 | 0,017 |
| Os4+ | \*DS | 30,4190 | 1,37113 | 15,2637 | 6,84706 | 14,7458 | 0,165191 | 5,06795 | 18,0030 | 6,49804 | 0,006 | 0,29 | 0,003 |
| Ir | \*RHF | 27,3049 | 1,59279 | 16,7296 | 8,86553 | 15,6115 | 0,417916 | 5,83377 | 45,0011 | 11,4722 | 0,050 | 0,09 | 0,017 |
| Ir3+ | \*DS | 30,4156 | 1,34323 | 15,8620 | 7,10909 | 13,6145 | 0,204633 | 5,82008 | 20,3254 | 8,27903 | 0,009 | 0,28 | 0,004 |
| Ir4+ | \*DS | 30,7058 | 1,30923 | 15,5512 | 6,71983 | 14,2326 | 0,167252 | 5,53672 | 17,4911 | 6,96824 | 0,006 | 0,29 | 0,003 |
| Pt | \*RHF | 27,0059 | 1,51293 | 17,7639 | 8,81174 | 15,7131 | 0,424593 | 5,78370 | 38,6103 | 11,6883 | 0,046 | 0,10 | 0,016 |
| Pt2+ | \*DS | 29,8429 | 1,32927 | 16,7224 | 7,38979 | 13,2153 | 0,263297 | 6,35234 | 22,9426 | 9,85329 | 0,014 | 0,00 | 0,006 |
| Pt4+ | \*DS | 30,9612 | 1,24813 | 15,9829 | 6,60834 | 13,7348 | 0,168640 | 5,92034 | 16,9392 | 7,39534 | 0,006 | 0,14 | 0,003 |
| Au | RHF | 16,8819 | 0,461100 | 18,5913 | 8,62160 | 25,5582 | 1,48260 | 5,86000 | 36,3956 | 12,0658 | 0,045 | 0,10 | 0,015 |
| Au1+ | \*DS | 28,0109 | 1,35321 | 17,8204 | 7,73950 | 14,3359 | 0,356752 | 6,58077 | 26,4043 | 11,2299 | 0,023 | 0,12 | 0,009 |
| Au3+ | \*DS | 30,6886 | 1,21990 | 16,9029 | 6,82872 | 12,7801 | 0,212867 | 6,52354 | 18,6590 | 9,09680 | 0,009 | 0,14 | 0,004 |
| Hg | RHF | 20,6809 | 0,545000 | 19,0417 | 8,44840 | 21,6575 | 1,57290 | 5,96760 | 38,3246 | 12,6089 | 0,046 | 0,10 | 0,017 |
| Hg1+ | \*DS | 25,0853 | 1,39507 | 18,4973 | 7,65105 | 16,8883 | 0,443378 | 6,48216 | 28,2262 | 12,0205 | 0,027 | 0,12 | 0,011 |
| Hg2+ | \*DS | 29,5641 | 1,21152 | 18,0600 | 7,05639 | 12,8374 | 0,284738 | 6,89912 | 20,7482 | 10,6268 | 0,013 | 0,00 | 0,006 |
| Tl | \*RHF | 27,5446 | 0,655150 | 19,1584 | 8,70751 | 15,5380 | 1,96347 | 5,52593 | 45,8149 | 13,1746 | 0,059 | 0,09 | 0,021 |
| T11+ | \*DS | 21,3985 | 1,47110 | 20,4723 | 0,517394 | 18,7478 | 7,43463 | 6,82847 | 28,8482 | 12,5258 | 0,028 | 0,12 | 0,011 |
| T13+ | \*DS | 30,8695 | 1,10080 | 18,3481 | 6,53852 | 11,9328 | 0,219074 | 7,00574 | 17,2114 | 9,80270 | 0,008 | 0,01 | 0,004 |
| Pb | RHF | 31,0617 | 0,690200 | 13,0637 | 2,35760 | 18,4420 | 8,61800 | 5,96960 | 47,2579 | 13,4118 | 0,060 | 2,00 | 0,021 |
| Pb2+ | \*DS | 21,7886 | 1,33660 | 19,5682 | 0,488383 | 19,1406 | 6,77270 | 7,01107 | 23,8132 | 12,4734 | 0,020 | 2,00 | 0,008 |
| Pb4+ | \*DS | 32,1244 | 1,00566 | 18,8003 | 6,10926 | 12,0175 | 0,147041 | 6,96886 | 14,7140 | 8,08428 | 0,005 | 0,31 | 0,002 |
| Bi | RHF | 33,3689 | 0,704000 | 12,9510 | 2,92380 | 16,5877 | 8,79370 | 6,46920 | 48,0093 | 13,5782 | 0,065 | 2,00 | 0,020 |
| Bi3+ | \*DS | 21,8053 | 1,23560 | 19,5026 | 6,24149 | 19,1053 | 0,469999 | 7,10295 | 20,3185 | 12,4711 | 0,015 | 2,00 | 0,006 |
| Bi5+ | \*DS | 33,5364 | 0,916540 | 25,0946 | 0,39042 | 19,2497 | 5,71414 | 6,91555 | 12,8285 | -6,7994 | 0,003 | 0,00 | 0,001 |
| Po | \*RHF | 34,6726 | 0,700999 | 15,4733 | 3,55078 | 13,1138 | 9,55642 | 7,02588 | 47,0045 | 13,6770 | 0,066 | 2,00 | 0,018 |
| At | \*RHF | 35,3163 | 0,685870 | 19,0211 | 3,97458 | 9,49887 | 11,3824 | 7,42518 | 45,4715 | 13,7108 | 0,062 | 2,00 | 0,015 |
| Rn | RHF | 35,5631 | 0,663100 | 21,2816 | 4,06910 | 8,00370 | 14,0422 | 7,44330 | 44,2473 | 13,6905 | 0,054 | 2,00 | 0,012 |
| Fr | \*RHF | 35,9299 | 0,646453 | 23,0547 | 4,17619 | 12,1439 | 23,1052 | 2,11253 | 150,645 | 13,7247 | 0,055 | 2,00 | 0,017 |
| Ra | \*RHF | 35,7630 | 0,616341 | 22,9064 | 3,87135 | 12,4739 | 19,9887 | 3,21097 | 142,325 | 13,6211 | 0,037 | 2,00 | 0,012 |
| Ra2+ | \*DS | 35,2150 | 0,604909 | 21,6700 | 3,57670 | 7,91342 | 12,6010 | 7,65078 | 29,8436 | 13,5431 | 0,029 | 2,00 | 0,006 |
| Ac | \*RHF | 35,6597 | 0,589092 | 23,1032 | 3,65155 | 12,5977 | 18,5990 | 4,08655 | 117,020 | 13,5266 | 0,030 | 0,06 | 0,009 |
| Ac3+ | \*DS | 35,1736 | 0,579689 | 22,1112 | 3,41437 | 8,19216 | 12,9187 | 7,05545 | 25,9443 | 13,4637 | 0,021 | 2,00 | 0,004 |
| Th | \*RHF | 35,5645 | 0,563359 | 23,4219 | 3,46204 | 12,7473 | 17,8309 | 4,80703 | 99,1722 | 13,4314 | 0,031 | 0,07 | 0,008 |
| Th4+ | \*DS | 35,1007 | 0,555054 | 22,4418 | 3,24498 | 9,78554 | 13,4661 | 5,29444 | 23,9533 | 13,3760 | 0,014 | 2,00 | 0,002 |
| Pa | \*RHF | 35,8847 | 0,547751 | 23,2948 | 3,41519 | 14,1891 | 16,9235 | 4,17287 | 105,251 | 13,4287 | 0,033 | 0,06 | 0,010 |
| u | RHF | 36,0228 | 0,529300 | 23,4128 | 3,32530 | 14,9491 | 16,0927 | 4,18800 | 100,613 | 13,3966 | 0,035 | 0,07 | 0,010 |
| u3+ | \*DS | 35,5747 | 0,520480 | 22,5259 | 3,12293 | 12,2165 | 12,7148 | 5,37073 | 26,3394 | 13,3092 | 0,009 | 2,00 | 0,002 |
| u4+ | \*DS | 35,3715 | 0,516598 | 22,5326 | 3,05053 | 12,0291 | 12,5723 | 4,79840 | 23,4582 | 13,2671 | 0,007 | 2,00 | 0,001 |
| u6+ | \*DS | 34,8509 | 0,507079 | 22,7584 | 2,89030 | 14,0099 | 13,1767 | 1,21457 | 25,2017 | 13,1665 | 0,003 | 2,00 | 0,001 |
| Np | \*RHF | 36,1874 | 0,511929 | 23,5964 | 3,25396 | 15,6402 | 15,3622 | 4,18550 | 97,4908 | 13,3573 | 0,037 | 0,07 | 0,011 |
| Np3+ | \*DS | 35,7074 | 0,502322 | 22,6130 | 3,03807 | 12,9898 | 12,1449 | 5,43227 | 25,4928 | 13,2544 | 0,006 | 2,00 | 0,002 |
| Np4+ | \*DS | 35,5103 | 0,498626 | 22,5787 | 2,96627 | 12,7766 | 11,9484 | 4,92159 | 22,7502 | 13,2116 | 0,005 | 2,00 | 0,001 |
| Np6+ | \*DS | 35,0136 | 0,489810 | 22,7286 | 2,81099 | 14,3884 | 12,3300 | 1,75669 | 22,6581 | 13,1130 | 0,002 | 2,00 | 0,001 |
| Pu | \*RHF | 36,5254 | 0,499384 | 23,8083 | 3,26371 | 16,7707 | 14,9455 | 3,47947 | 105,980 | 13,3812 | 0,038 | 0,14 | 0,013 |
| Pu3+ | \*DS | 35,8400 | 0,484938 | 22,7169 | 2,96118 | 13,5807 | 11,5331 | 5,66016 | 24,3992 | 13,1991 | 0,005 | 2,00 | 0,001 |
| Pu4+ | \*DS | 35,6493 | 0,481422 | 22,6460 | 2,89020 | 13,3595 | 11,3160 | 5,18831 | 21,8301 | 13,1555 | 0,003 | 2,00 | 0,001 |
| Pu6+ | \*DS | 35,1736 | 0,473204 | 22,7181 | 2,73848 | 14,7635 | 11,5530 | 2,28678 | 20,9303 | 13,0582 | 0,001 | 1,36 | 0,001 |
| Am | \*RHF | 36,6706 | 0,483629 | 24,0992 | 3,20647 | 17,3415 | 14,3136 | 3,49331 | 102,273 | 13,3592 | 0,040 | 0,07 | 0,013 |
| Cm | \*RHF | 36,6488 | 0,465154 | 24,4096 | 3,08997 | 17,3990 | 13,4346 | 4,21665 | 88,4834 | 13,2887 | 0,041 | 0,07 | 0,013 |
| Bk | \*RHF | 36,7881 | 0,451018 | 24,7736 | 3,04619 | 17,8919 | 12,8946 | 4,23284 | 86,0030 | 13,2754 | 0,042 | 0,07 | 0,014 |
| Cf | \*RHF | 36,9185 | 0,437533 | 25,1995 | 3,00775 | 18,3317 | 12,4044 | 4,24391 | 83,7881 | 13,2674 | 0,043 | 0,07 | 0,014 |