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Fortran90 sources of the subroutines of *UMWEG*. I. The subroutine *UPFORM* for the determination of dispersion corrections and scattering-factors for free atoms and ions

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The Fortran90 source of the subroutine *UPFORM*, which provides dispersion corrections and scattering factors for all free atoms and ions in the range $0 \leq \sin\theta/\lambda \leq 6$ Å^{-1}, has been deposited in the IUCr electronic archives.

1. Introduction

As pointed out by Waasmaier & Kirfel (1995), the parameters of some of the atoms and ions given in Table 6.1.1.4, for $0 \leq \sin\theta/\lambda \leq 2$ Å^{-1}, and Table 6.1.1.5, for $2 \leq \sin\theta/\lambda \leq 6$ Å^{-1} (where θ is the Bragg angle and λ is the wavelength), of the *International Tables of Crystallography* (1992), Vol. C, which are used for scattering-factor calculation in the program *UMWEG* (Rossmanith, 2006, 2003), do not fit the scattering factors of Table 6.1.1.1 for atoms and Table 6.1.1.3 for ions, even after correction of the apparent misprints in Table 6.1.1.1 for P at 2.5 Å^{-1} ($f = 1.122$), Se at 3.5 Å^{-1} ($f = 2.108$) and Am at 3.5 Å^{-1} ($f = 11.095$). Waasmaier & Kirfel (1995) therefore developed a new analytical scattering-factor representation valid for the full range from 0.0 to 6.0 Å^{-1}. On the other hand, it is shown in the following that satisfactory agreement between the scattering factors $f(\sin\theta/\lambda)$ given in the Tables 6.1.1.1 and 6.1.1.3 and the results of the representation

$$f(\sin\theta/\lambda) = \sum_{i=1}^{4} a_i \exp\left[-b_i(\sin\theta/\lambda)^2\right] + c, \qquad (1)$$

calculated with the parameters a_i, b_i and c, collated in Table 6.1.1.4, in combination with the representation

$$\ln[f(\sin\theta/\lambda)] = \sum_{i=0}^{3} a_i(\sin\theta/\lambda)^i, \qquad (2)$$

calculated with the parameters a_i, collated in the Table 6.1.1.5, is obtained, modifying few of the parameters given in the latter two Tables and modifying the range of validity of the equations (1) and (2) for some ions.

2. Modifications of Tables 6.1.1.4 and 6.1.1.5

In the work of Rossmanith (1999), the modifications used in *UMWEG* for Mg, Si, Ni and Zr were given. Unfortunately there is a misprint in that paper: the parameters of Table 6.1.1.5 that have to be replaced are a_0 and a_3 instead of a_0 and a_2 (see file `IT_Table_6.1.1.5.txt` for the modified Table 6.1.1.5, and `fig_2.ps` in the deposited material[1]). Apart from the corrections of the parameters of Table 6.1.1.5, two misprints in Table 6.1.1.4 were found: for Ru^{4+}, the parameter b_3 has to be replaced by 0.036495, and for Bi^{5+}, the parameter b_2 has to be replaced by 0.039042 (see deposited material, file `IT_Table_6.1.1.4.txt`, for the modified Table 6.1.1.4). In Fig. 1, the results obtained with the unmodified parameters (left-hand diagrams) are compared with those obtained with the modified parameters (right-hand diagrams).

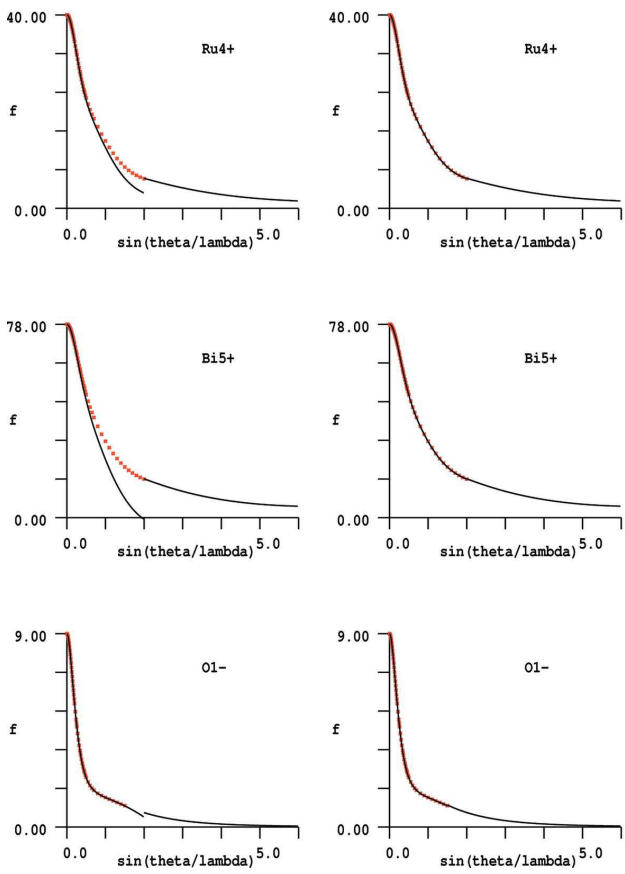

Figure 1
Comparison of the scattering factors given in the Table 6.1.1.3 (red crosses) with those obtained with the unmodified (left-hand diagrams) and modified (right-hand diagrams) Tables 6.1.1.4 and 6.1.1.5 for Ru^{4+} and Bi^{5+}. In the case of O^{1-}, the left (right) diagram shows the comparison for the unmodified (modified) range of validity of the equations (1) and (2).

[1] Supplementary data for this paper are available from the IUCr electronic archives (Reference: cg5050). Services for accessing these data are described at the back of the journal.

3. The Fortran source of the *UMWEG* subroutine *UPFORM*

Together with the dispersion corrections for Cu, Mo and Ag radiation [*International Tables of Crystallography* (1992), Vol. C, pp. 219–222], the modified Tables 6.1.1.4 and 6.1.1.5 are incorporated in the subroutine *UPFORM* as DATA statements (see deposited material, file `upform.f90`). The parameters given in Table 6.1.1.5 for atoms only, are also used for the corresponding ions (Waasmaier & Kirfel, 1995). The subprogram searches the appropriate values from these DATA statements.

Because of the problems found with the range of validity of equation (1) for O^{1-}, F^{1-}, Sc^{3+}, Ti^{2+}, Ti^{3+}, Ti^{4+} and V^{3+}, for these ions the range of validity of equations (1) and (2) is modified. In Fig. 1, it is demonstrated for O^{1-}, as an example, that satisfactory fits for these ions can be obtained, using equation (1) in the range $0 < \sin\theta/\lambda \leq 1.5$ Å^{-1}, and equation (2) otherwise.

The graphical representation of the comparison of the scattering factors obtained with the modified Tables 6.1.1.1 and 6.1.1.3 with those obtained with the values given in the UPFORM-DATA statements for all atoms and ions can be copied from the deposited material (files `fig.ps`, `IT_Table_6.1.1.1.txt` and `IT_Table_6.1.1.3.txt`).

References

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