International Union of Crystallography


**International Tables for Crystallography**

*Volume C: Mathematical, Physical and Chemical Tables*

Edited by A. J. C. Wilson

Reprinted with corrections and additions 1995

Corrigenda and Addenda to the First Edition (1992)

A corrected reprint of *International Tables for Crystallography*

*Volume C* was published in February 1995. Corrections and additions to the First Edition are listed below.

Page Additions to the First Edition are listed below.

9.6

F. H. ALLEN: Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England. [9.5, 9.6]

P. J. BECKER: Département de Sciences des Matériaux, Université de Marne la Vallée, 2 Allée Jean Renoir, 93160 Noisy le Grand, France. [8.7]

S. ĐUROVIĆ: Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta, 842 36 Bratislava, Slovakia. [9.2.2]

E. GALDECKA: Institute of Low Temperature and Structure Research PAS, 50-950 Wroclaw 2, PO Box 937, Poland. [5.3]

O. KENNARD: Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England. [9.5, 9.6]

E. GALDECKA: Institute of Low Temperature and Structure Research PAS, 50-950 Wroclaw 2, PO Box 937, Poland. [5.3]

O. KENNARD: Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England. [9.5, 9.6]

Add the following:

K. BRANDENBURG: Anorganisch-chemisches Institut der Universität Bonn, D-5300 Bonn, Gerhard-Domagkstrasse 1, Germany. [9.4]


†C. H. MACGILLAVRY. [3.1]

A. OLSSEN: Centre for Materials Research, University of Oslo, N-0371 Oslo, Norway. [5.4.2]

R. PYNN: Los Alamos National Laboratory, PO Box 1663, LANSCe, MS H805, Los Alamos, NM 87545, USA. [4.4.3]

J. M. ROWE: National Institute of Science and Technology, Reactor Research Division, Gaithersburg, MD 20899, USA. [4.4.3]

T. M. SABINE: ANSTO, Private Mail Bag 1, Menai, New South Wales 2234, Australia. [6.4]

N. J. TIGHE: 104 Surfview Drive #1501, Palm Coast, FL 32137, USA. [3.5]

V. VALVODA: Department of Physics of Semiconductors, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Praha 2, Czech Republic. [4.1]

D. G. WATSON: Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, England. [9.5, 9.6]

A. J. C. WILSON: St John’s College, Cambridge CB2 1TP, England. [1.4, 4.2.5, 5.1, 5.2, 7.5, 9.7]

B. B. ZVYAGIN: Institute of Ore Mineralogy, Akad. Nauk Russia, Staromonetnaya 35, 109017 Moscow, Russia. [4.3.5]

Add the following:

V. H. SMITH JR: Department of Chemistry, Queen’s University, Kingston, Ontario K7L 3N6, Canada. [4.3.3]

J. WANG: Department of Chemistry, Queen’s University, Kingston, Ontario K7L 3N6, Canada. [4.3.3]

Add “J. Wang and V. H. Smith Jr” to author list for Section 4.3.3.

Add “K. Brandenburg” to author list for Section 9.4.

Table 1.4.2 (cont.), delete second “4m” in the second column.

20 At the end of the section “Patterson symmetry in the dispersive case”, add “An alternative description of such symmetries, in terms of seventy-three of the 1651 dichromatic colour groups, has been given by Fischer & Knof (1987); see also Wilson (1993).”

20 Add the following references to the reference list:


Note (4). Change “turned” to “tuned”.

Left column, line 22, change “reflections for film” to “reflections per film”.

Left column, line 25, change “Parrett” to “Parratt”.

Right column, line 37, change “n(n−10)” to “4n−10 for n > 3”.

Left column, line 19, change “PARRETT” to “PARRATT”.

Section 4.3.3, add “J. Wang and V. H. Smith Jr” to list of authors.

Left column, line 13, change “Theusen” to “Thuesen”.

Table 4.2.3.1, change address for Photon Factory to “National Laboratory for High Energy Physics, 1-1 Oho, Tsukuba-gun, Ibaraki 305, Japan”.

Delete note of “Note added in proof”. Replace with:

“Note added in proof. A workshop on standards and criteria in XAFS spectroscopy was held at Brookhaven National Laboratory under the co-chairmanship of F. W. Lytle, D. E. Sayers and E. A. Stern in May, 1988 [Physica B, 158, 701–722]. This meeting set up a Standards and Criteria Committee under the direction of D. Koningsberger, which reported its findings to the XAFS meeting in Kobe [Jpn. J. Appl. Phys. 32, Suppl. 32-2, 877–878]. It must be stressed that the use of computer programs based on the plane-wave theory should be discouraged, and that programs based on the curved-wave theories should always be used in analyses. Furthermore, multiple scattering should be considered routinely in the analysis of data.”

In addition, the XAFS community adopted a new, more formal, organization, and is now the International XAFS Society (IXS).”

Right column, line 36, change “were” to “are”.

Equation (4.2.4.6), delete factor “2”;

Equation (4.2.4.9), insert parentheses around “cos φ”.

Transpose Figs. 4.2.4.1 and 4.2.4.3.
Right column, line after equation (4.2.6.1), delete "\( \frac{e}{mc^2} \)".
Equation (4.2.6.2), replace "\( \cdot r^n \)" with "\( \cdot r \)".
Equation (4.2.6.4), delete factor "\( 4\pi \)".
Right column, line 5, replace "\( \varepsilon \)" with "\( \varepsilon_0 \)".
Equation (4.2.6.6), replace limit "\( n = 2 \)" by "\( n = Z \)".
Left column, line 17, change "\( F(x, Z) \)" to "\( F(x, Z) \)".
Left column, line 20, change "\( A/2\pi r \)" to "\( A/4\pi r \)".
Left column, line 16, change "superceded" to "superseded".
Equation (4.2.6.9), change first "-" sign to "+" sign.
Equation (4.2.6.11), replace with
\[
 f' = \int_0^\infty \frac{\omega'^2 (d\varepsilon_\alpha/d\omega')}{\omega'^2 - \omega^2} d\omega.
\]
Equation (4.2.6.12), replace with
\[
 f' = \sum_\kappa \int_0^\infty \frac{\omega^2 (d\varepsilon_\alpha/d\omega')}{\omega^2 - \omega'^2} d\omega.
\]
Equation (4.2.6.13), replace with
\[
 \mu_\alpha = \frac{2\pi e^2}{\varepsilon_0 mc} \left[ \frac{d\varepsilon}{d\omega} \right].
\]
Equation (4.2.6.14), replace with
\[
 f'' = \frac{\pi}{2} \left[ \frac{d\varepsilon_\alpha}{d\omega} \right].
\]
Equation (4.2.6.15), replace with
\[
 f' = \frac{2}{\pi} \sum_\kappa P \int_0^\infty \frac{\omega' f''(\omega', 0)}{\omega^2 - \omega'^2} d\omega'.
\]
Equation (4.2.6.22), replace with
\[
 f'(\omega, 0) = \frac{2}{\pi} P \int_0^\infty \frac{\omega' f''(\omega', 0)}{\omega^2 - \omega'^2} d\omega'.
\]
Right column, line 28, change "\( 1 + ik \cdot r \)" to "\( 1 - ik \cdot r \)".
Right column, line 14, change "\( f'(\omega, 0) \)" to "\( f'(\omega, 0) \)".
Equation (4.2.6.25), change "\( f'(\omega, 0) \)" to "\( f'(\omega, 0) \)".
Fig. 4.2.6.2(a), replace "\( f'(\omega, 0) \)" by "\( f'(\omega, 0) \)".
Left column, line 16, change "Theussen" to "Theusen".
Right column, line 4, change "1992" to "1993".
Right column, line 6, change "Kato" to "Kato".
Right column, line 3, change "+0.25" to "+0.20".
Right column, line 4, change "-0.25" to "-0.10".
Table 4.2.6.7, change "Argawal" to "Agrawal" in heading.
Table 4.2.6.8, change "fp" to "f'" and "fpp" to "f''".
Table 4.2.6.8 (cont.), change "fp" to "f'" and "fpp" to "f''".
Table 4.2.6.8 (cont.), change "Ee" to "Ee".
Table 4.2.6.8 (cont.), change "fp" to "f'" and "fpp" to "f''".

Table 4.2.6.8 (cont.), for Th, change first "fp" to "f'" and second "fp" to "f''".
Table 4.2.6.8 (cont.), change "fp" to "f'" and "fpp" to "f''".
Right column, line 7, change "0.83" to "0.81".
Right column, after line 10 add: "

Correction term
\( (E_{tot}/mc^2) \)
\[
\begin{array}{cccc}
Z & 0.99 & 0.99 & 0.99 \\
6 & 0.99 & 0.94 & 0.93 \\
10 & 0.91 & 0.90 & 0.86 \\
14 & 0.84 & 0.82 & 0.81
\end{array}
\]

I am indebted to Dr C. G. Cousins for his helpful comments regarding the exposition of the non-relativistic theory in the 1992 printing of this section. I have modified the text of the current printing according to his suggestions. The nomenclature is now consistent with standard works on the non-relativistic scattering of X-rays by isolated atoms."

Section 4.3.3, add "J. Wang and V. H. Smith Jr" to list of authors.
Right column, change third equation to
\[
\alpha = \frac{e^2}{\hbar c}.
\]
Right column, after second equation, replace "The function ... Cromer, 1969)." with "The function \( S(s) \) is the X-ray incoherent scattering factor (Wang, Sagar, Schmider & Smith, 1993) and is related to the inelastic electron scattering cross section by
\[
\sigma_{inel}(s) = 4S(s)/a^2 s^4.
\]

Inelastic scattering factors for X-rays and electrons are given in Table 4.3.3.2 in the Morse (1932) approximation for elements \( Z = 1 \) to \( Z = 90 \) with HF wave functions (Bunge, Barrientos & Bunge, 1993; McLean & McLean, 1981)."

Table 4.3.3.2 has been replaced by a new table. Purchasers of the First Edition may obtain free copies of this table from The Technical Editor, IUCr, 5 Abbey Square, Chester CH1 2HU, England.
363 Equation (4.3.7.2a), change “$z^2$” to “$z_{g}^2$”.
Equation (4.3.7.2b), change “$(\gamma_1 - \gamma_2 )^2$” to “$(\gamma_{1g} - \gamma_{2g} )^2$”.
402 Right column, line 4, change “THEUSSEN” to “THUESEN”.
405 Left column, Section 4.2.6 references, line 11, change “ARGAWAL” to “AGARWAL”.
406 Right column, line 4, change “THEUSSEN” to “THUESEN”.
407 Left column, line 15, change “1992” to “1993”.
409 Right column, line 4, change “THEUSSEN” to “THUESEN”.
410 Right column, line 44, change “THEUSSEN” to “THUESEN”.
411 Right column, line 4, change “THEUSSEN” to “THUESEN”.
412 Left column, line 15, change “1992” to “1993”.
413 Left column, line 15, change “1992” to “1993”.
414 Right column, line 44, change “THEUSSEN” to “THUESEN”.
415 Right column, line 4, change “THEUSSEN” to “THUESEN”.
416 Right column, line 4, change “THEUSSEN” to “THUESEN”.
417 Left column, line 15, change “1992” to “1993”.
418 Right column, line 44, change “THEUSSEN” to “THUESEN”.
419 Right column, line 4, change “THEUSSEN” to “THUESEN”.
420 Right column, line 4, change “THEUSSEN” to “THUESEN”.
421 Right column, line 4, change “THEUSSEN” to “THUESEN”.
422 Right column, line 22, change “Welch” to “Welsch”.
Equation (8.7.2.4), delete commas after “$a_1$” and “$a_2$”.
Equation (8.7.3.20b), replace “$a_r$” with “$a_{r_2}$”.
Line –9, change “Coppens, 1992” to “Coppens, 1993”.
Equation (8.7.3.21b), replace with
\[
Q_{xx} = \frac{1}{2} P_{20} \frac{30}{\zeta^3} \frac{L_{20}}{(M_{20})^2} = \frac{18\sqrt{3}}{\zeta^3} P_{20}
\]
and
\[
Q_{\alpha\beta} = \frac{9\pi}{\zeta} P_{\text{tmp}}.
\]
Equation (8.7.3.25), replace with
\[
Q_{\alpha\beta} = Q_{\alpha\beta} + \frac{1}{2} \left( 3\rho'_{r_2} r_{2\beta} - r_2^2 \delta_{r_2\beta} \right) q
\]
\[
- \frac{3}{2} \left( r_{2\beta} \mu_\alpha + r_{2\beta} \mu_\beta \right) + \left( \sum_r r_{2\beta} \mu_\alpha \right) \delta_{r_2\beta}.
\]
631 Table 8.7.3.2, replace entries in third column by
\[
V_{7} j_0(2\pi h_{\gamma} \delta_{\gamma}) j_0(2\pi h_{\gamma} \delta_{\gamma}) j_0(2\pi h_{\gamma} \delta_{\gamma})
\]
for $\gamma = 1$.
\[\begin{align*}
-iv_{\gamma} \delta_{\alpha} j_1(2\pi h_{\gamma} \delta_{\gamma}) \\
&\times j_0(2\pi h_{\gamma} \delta_{\gamma}) j_0(2\pi h_{\gamma} \delta_{\gamma})
\end{align*}\]
for $\gamma = r_{1\gamma}$.
\[\begin{align*}
-iv_{\gamma} \delta_{\beta} j_1(2\pi h_{\gamma} \delta_{\gamma}) j_0(2\pi h_{\gamma} \delta_{\gamma}) \\
&\times j_1(2\pi h_{\gamma} \delta_{\beta}) j_0(2\pi h_{\gamma} \delta_{\gamma})
\end{align*}\]
for $\gamma = r_{2\gamma}$.
Equation (8.7.3.32), change first “–” sign in second line of equation to “*” sign.
Replace first two lines of equation (8.7.3.33) with
\[
\nabla E_{11} = + (3/5) \left( \pi P_{22} + 3/2 P_{20} \right) Q_r
\]
\[
\nabla E_{22} = - (3/5) \left( \pi P_{22} + 3/2 P_{20} \right) Q_r
\]
Equation following equation (8.7.3.33), replace “$R(r)$” with “[R(r)]$\ast$”.
Equation (8.7.3.34), change “$1/2$” to “$1/2$”.
632 Left column, line 1, change “$V_{\gamma\alpha}$” to “$Q_{\gamma\alpha}$”.
Left column, line 23, replace “for the electronic charge distribution” with “for a charge distribution”.
Equation (8.7.3.39a), change “$V^2$” to “$V^\ast$”.
Right column, line 11, change “may” to “must”.
Equation (8.7.3.39b), change “$V^2$” to “$V^\ast$”.
634 Table 8.7.3.5, footnote *, replace “$e'_{\gamma} = \sqrt{2/3} d_{\gamma}$” with “$e'_{\gamma} = \sqrt{1/3} d_{\gamma} - \sqrt{2/3} d_{\gamma}$”.
645 Equation (8.8.3a), change “$s^2$” to “$s_2^\ast$”.
649 References to Section 8.2, line 1, change “WELCH” to “WELSCH”.
650 References to Section 8.5, line 6, change “WELCH” to “WELSCH”.


671 Right column, line 12, remove comma after “conditions”.

673 Right column, line -17, change “Subsection” to “§”.

674 Left column, line -22, change “the USSR” to “the former USSR”.

678 Fig. 9.2.2.16, replace the following labels: “24” below 26 with “24”, “33” below 06 with “33”, “33” below 06 with “33”, “33” below 06 with “33”, “21” below 26 with “24”, “36” below 39 with “36”. Right column, line -3, change “2/m” to “2/1/m”.

679 Left column, line 14, change “P(m)cn” to “P(m)cm”.

680 Right column, delete last paragraph.

683 Section 9.4, add “K. Brandenburg” to list of authors. Left column, lines 14–17, replace with “Inorganic Crystal Structure Database (ICSD) (Bergerhoff & Brown, 1987) this analysis has been performed with the 1990 version for all combinations of ions and atoms; 8876 sets of data were calculated. The procedure is described in the following paragraphs and a short list of examples is given in Table 9.4.2.1. The full information is contained in the CD-ROM version of the ICSD, from which the distribution of distances for any ion pair can be displayed.”

792 Right column, line 3, missing symbol should be “x_i”. Right column, line 32, replace “two (P3 and R3) of the four” with “three (P1, P3, R3) of the five”.


840 Delete reference “SCHRAUBER, FICHTNER, GRELL & WINTER (1987)”.

841 References to Section 9.2.2, reference “TSVETKOV (1982)”, add “[In Russian.]”.

851 Table 10.3.1, delete entry for Germany, Democratic Republic. Belgium entry, change “Controles” to “Contrôles”. Replace entry for Czechoslovakia with “Czech Republic; Legislation: Communications of Ministry of Health of ČSR (1972) / Czechoslovak State Norm No. 341725 (1968); Proclaimed: —; Responsible authority: Institute of Physics, Academy of Sciences of the Czech Republic, 18040 Prague 8, Na Slovance 2”. France entry, change “Fédération” to “Fédération”. Table 10.3.1 (cont.), Germany, Federal Republic of entry, change “Verordnung” to “Verordnung”, change “13/10/76” to “13/10/78”, change “—” to “8/1/87”.

853 Table 10.3.1 (cont.), Singapore entry, change “Ontram” to “Outram”; insert entry “Slovak Republic; Legislation: Act of the Ministry of Health of the Slovak Socialist Republic No. 65 / Czechoslovak State Norm No. 451725; Proclaimed: 12/9/72 / 24/7/68; Responsible authority: Ministry of Health of the Slovak Republic, Limbová 2, SK-83341 Bratislava.”. Switzerland entry, change “Office Federal de la Santé Publique” to “Office Fédéral de la Santé Publique.”

855 Change “Argawal, B.K.” to “Agarwal, B.K.”; add “Barrientos, J., 4.3.3.”

856 Add “Brandenburg, K., 9.4”; add “Brese, N.E., 9.1”; add “Bunge, A.V., 4.3.3.”; delete “4.3.3” for “Cromer, D.T.”.

857 Delete “Fichtner, K., 9.2.2”; delete “George, J.B., 5.3.”

858 Delete “Grell, H., 9.2.2.”.

860 Change “Marsch, P.” to “Marsh, P.”; add “4.3.3” to “McLean, A.D.”; add “McLean, R.S., 4.3.3.”

861 Delete “Nicolas, D., 4.3.3”; add “2.3” to “Parratt, L.G.”; delete “Parratt, L.G., 2.3”.

862 Delete “Roualt, M., 4.3.3”; add “Sagar, R.P., 4.3.3”; add “Schmider, H., 4.3.3”; delete “2.3” for “Schrauber, H.”; delete “Schuttke, G.H.”; add “5.3” to “Schuttke, G.H.”

863 Add “Skov Pedersen, J.; see Pedersen, J.S.”; add “6.1.1” to “Smith, V.H.”; change “Theussen, G.” to “Thuesen, G.”.

864 Add “Wang, J., 4.3.3”; delete “Welch, R.E., 8.2, 8.5”; add “8.2, 8.5” to “Welsch, R.E.”; delete “Winter, G., 9.2.2.”; delete “Wölfel, E., 7.1.6” to “Wölfel, E.R.”

869 Add “Colour groups, 20”.

875 Add “Molecular symmetry, 796”.

877 Add “Patterson synthesis, 20”.

881 Under “Symmetry” heading, add “molecular, 796”, “of Patterson synthesis, 20”, “Symmorphism, 796”.