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International Tables for Crystallography Volume C: Mathematical, Physical and Chemical Tables

Edited by A. J. C. Wilson

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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

vi

- v Replace original text with the following:
  - 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]

†L. D. CALVERT. [9.3]

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

E. GAŁDECKA: Institute of Low Temperature and Structure Research PAS, 50-950 Wrocław 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]

Replace original text with the following: P. F. LINDLEY: SERC Daresbury Laboratory, Warring-

ton WA4 4AD, England. [3.4] †C. H. MACGILLAVRY. [3.1]

A. OLSEN: 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, Staromonetny 35, 109017 Moscow, Russia. [4.3.5]

Add the following:

V. H. SMITH JR: Department of Chemistry, Queen's University, Kingston, Ontario K7I 3N6, Canada. [4.3.3] J. WANG: Department of Chemistry, Queen's University, Kingston, Ontario K7I 3N6, Canada. [4.3.3]

- xiv Add "J. Wang and V. H. Smith Jr" to author list for Section 4.3.3.
- xxv Add "K. Brandenburg" to author list for Section 9.4.
- 18 Table 1.4.2 (cont.), delete second " $\bar{4}m$ " 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: "FISCHER, K. F. & KNOF, W. E. (1987). Space groups for imaginary Patterson and for difference Patterson functions in the lambda technique. Z. Kristallogr. 180, 237-242.

WILSON, A. J. C. (1993). Laue and Patterson symmetry in the complex case. Z. Kristallogr. 208, 199–206."

- 25 Note (4). Change "turned" to "tuned".
- 33 Left column, line 22, change "reflections for film" to "reflections per film".
- 75 Left column, line 25, change "Parrett" to "Parratt".
- 111 Right column, line 37, change "n(n-10)" to "4n-10 for n > 3".
- 127 Left column, line 19, change "PARRETT" to "PARRATT".
- 161 Section 4.3.3, add "J. Wang and V. H. Smith Jr" to list of authors.
- 184 Left column, line 13, change "Theussen" to "Thuesen".
- 189 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 text 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".

- 190 Equation (4.2.4.6), delete factor "2".
- 191 Equation (4.2.4.9), insert parentheses around "cos  $\varphi$ ". Transpose Figs. 4.2.4.1 and 4.2.4.3.

- 207 Right column, line after equation (4.2.6.1), delete "=  $e^2/m_e c^2$ ". Equation (4.2.6.2), replace "]  $\cdot$  r" 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". 208
- Left column, line 17, change " $F(x_1Z)$ " to "F(x,Z)". Left column, line 20, change " $\Delta/2\pi$ " to " $\Delta/4\pi$ ". 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

$$f' = \int_{\omega_{\kappa}}^{\infty} \frac{\omega'^2 (\mathrm{d}g_{\kappa}/\mathrm{d}\omega')}{\omega^2 - \omega'^2} \mathrm{d}\omega$$

Equation (4.2.6.12), replace with

$$f' = \sum_{\kappa} \int\limits_{\omega_{\kappa}}^{\infty} rac{\omega'^2 (\mathrm{d}g_{\kappa}/\mathrm{d}\omega')}{\omega^2 - \omega'^2} \mathrm{d}\omega$$

Equation (4.2.6.13), replace with

$$\mu_a = rac{2\pi^2 e^2}{arepsilon_0 mc} iggl[ rac{\mathrm{d}g}{\mathrm{d}\omega} iggr].$$

Equation (4.2.6.14), replace with

$$f^{\prime\prime} = \frac{\pi}{2} \omega \left[ \frac{\mathrm{d}g_{\kappa}}{\mathrm{d}\omega} \right]$$

209 Equation (4.2.6.15), replace with

$$f' = \frac{2}{\pi} \sum_{\kappa} P \int_{\omega_{\kappa}}^{\infty} \frac{\omega' f''(\omega', 0)}{\omega^2 - {\omega'}^2} \mathrm{d}\omega'.$$

Equation (4.2.6.22), replace with

$$f'(\omega,0) = \frac{2}{\pi} P \int_{0}^{\infty} \frac{\omega' f''(\omega',0)}{\omega^2 - {\omega'}^2} \mathrm{d}\omega'$$

Right column, line 28, change " $1 + i\mathbf{k} \cdot \mathbf{r}$ " to " $1 - i\mathbf{k} \cdot \mathbf{r}$ ". Right column, line -14, change " $f'(\omega_1, 0)$ " to " $f'(\omega, 0)$ ".

- 210 Equation (4.2.6.25), change " $f'(\omega, 0)$ " to " $f^+(\omega, 0)$ ". 211 Fig. 4.2.6.2(*a*), replace "f'(-, 0)" by " $f(\omega, 0)$ ".
- Left column, line 16, change "Theussen" to "Thuesen". 215 Right column, line 4, change "1992" to "1993".
- 216
- Right column, line 6, change "Kato" to "Katoh". Right column, line 3, change "+0.25" to "+0.20". 219 Right column, line 4, change "-0.25" to "-0.10" Table 4.2.6.7, change "Argawal" to "Agarwal" 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 220 "f"".
  - Table 4.2.6.8 (cont.), change "Ee" to "Fe".
- Table 4.2.6.8 (cont.), change "fp" to "f'" and "fpp" to 221 "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 222 "f"".

Right column, line 7, change "0.83" to "0.81". Right column, after line 10 add: "

Z	Correction term $(E_{tot}/mc^2)$
6	0.99
10	0.99
14	0.99
20	0.94
30	0.93
40	0.91
50	0.90
60	0.86
70	0.84
80	0.82
90	0.81

Multiplication of the correction factor by the appropriate value for  $E_{tot}/mc^2$  will give the S-matrix result.

A comparison of the results of the RMP theory and experimental results is given by Creagh [Nucl. Instrum. Methods (1990), A295, 417-434].

The computer program for the RMP theory has been in use for six years and has proven to give excellent agreement with experiment for elements with atomic number as high as 92 (uranium), even in the neighbourhood of its K-absorption edge [Creagh: Indian J. Phys. (1993), 67B, 511-525; Acta Cryst. (1993), A49, 32].

I am indebted to Dr C. S. 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."

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

Right column, change third equation to

$$\alpha = \frac{e^2}{\hbar c}.$$

246 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

$$\sigma_{\rm inel}(s) = 4S(s)/a^2s^4.$$

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. 327 Purchasers of the First Edition may obtain free copies of this table from The Technical Editor, IUCr, 5 Abbey Square, Chester CH1 2HU, England.

- Equation (4.3.7.2*a*), change " $s^2$ " to " $s_g^2$ ". Equation (4.3.7.2*b*), change " $(\gamma^i \gamma^i)$ " to " $(\gamma^i \gamma^j)$ ". Right column, line 4, change "THEUSSEN" to "THUESEN". 363
- 402
- Left column, Section 4.2.6 references, line 11, change 405 "ARGAWAL" to "AGARWAL".
- Right column, line 1, change "HART, N." to "HART, M." Right column, line 44, change "THEUSSEN" to 406 "THUESEN".
- Left column, line 15, change "1992" to "1993". 407
- Delete reference to "CROMER (1969)", add the following 409 references:

"BUNGE, C. F., BARRIENTOS, J. & BUNGE, A. V. (1993). Roothaan-Hartree-Fock ground-state atomic wave functions: Slater-type orbital expansions and expectation values. Atomic Data Nucl. Data Tables, 53, 113-162.

MCLEAN, A. D. & MCLEAN, R. S. (1981). Roothaan-Hartree-Fock atomic wave functions: Slater basis-set expansions for Z = 55-92. Atomic Data Nucl. Data Tables, 26, 197-381."

- 410 Delete reference "TAVARD, NICOLAS & ROUAULT (1967)", add reference: "WANG, J., SAGAR, R. P., SCHMIDER, H. & SMITH, V. H. JR (1993). X-ray elastic and inelastic scattering factors for neutral atoms Z = 2-92. Atomic Data Nucl. Data Tables, 53, 233-269."
- 447 Equation (5.3.3.17), replace with

$$\sigma^2(\theta_{\rm mc}) = \sigma^2(\theta_i) + \sigma(h_i) / [h'(\theta_i)]^2.$$

Right column, line 36, replace " $F = F_{min} = 0.84375$ " with " $F = F_{\min} = 0.84$ ".

- References to Section 5.3, line 1, change "MARSCH" to 468 "Marsh".
- Left column, line 44, change "GEORGE, J. B." to 469 "GEORGE, J. D."
- 472 Left column, line 38, add "PAN" after "Strukturalnych". Right column, line 45, change "SCHUTTKE" "SCHWUTTKE".
- 477 Replace footnote with "† Thakkar & Smith (1992)."
- 488 Replace footnote with "† Thakkar & Smith (1992)."
- Table 6.1.1.5, replace "37 Pb" with "37 Rb", "41 No" with "41 Nb", "86 Pn" with "86 Rn", "88 Pa" with "88 Ra", "98 Cl" with "98 Cf". 503

Table 6.3.3.2: 523  $\theta$ =30°,  $\mu$ R=1.5, change "8.320" to "8.230"  $\theta$ =40°,  $\mu$ R=1.0, change "4.4261" to "4.2461"  $\theta$ =75°,  $\mu$ R=1.7, change "5.4799" to "5.7499". Table 6.3.3.3:  $\theta$ =40°,  $\mu$ R=0.9, change "3.3208" to "3.2308"

- $\theta$ =75°,  $\mu R$ =0.6, change "1.1256" to "2.1257". Table 6.3.3.4:
- $\theta$ =65°,  $\mu R$ =0.7, change "1.0025" to "1.0250"  $\theta$ =60°,  $\mu R$ =2.2, change "0.3098" to "0.5098". 534 References for Section 6.1.1, add

524

- "THAKKAR, A. J. & SMITH, V. H. JR (1992). Highaccuracy ab-initio form factors for the hydride anion and isoelectronic species. Acta Cryst. A48, 70-71."
- 574 Table 7.4.3.1, replace caption with "The energy transfer, in eV, in the Compton scattering process for selected X-ray energies".
- 587 References to Section 7.1.6, change "WÖLFEL, E. (1983)" to "WÖLFEL, E. R. (1983)".
- Right column, line 24, change "Welch" to "Welsch". 606

- Right column, line 22, change "Welch" to "Welsch". 622
- 627 Equation (8.7.2.4), delete commas after " $ds_1$ " and "d2".
- Equation (8.7.3.20b), replace " $\alpha^l$ " with " $\zeta'$ ". Line -9, change "Coppens, 1992" to "Coppens, 1993". 630 Equation (8.7.3.21b), replace with

$$Q_{xx} = \frac{1}{2} P_{20} \cdot \frac{30}{\zeta^2} \frac{L_{20}}{(M_{20})^2} = \frac{18\sqrt{3}}{\zeta^2} P_{20}$$

and

$$Q_{\alpha\beta} = \frac{9\pi}{\zeta^2} P_{lmp}.$$

Equation (8.7.3.25), replace with

$$\begin{aligned} Q'_{\alpha\beta} &= Q_{\alpha\beta} + \frac{1}{2} \left( 3r'_{\alpha}r'_{\beta} - r'^{2}\delta_{\alpha\beta} \right) q \\ &- \frac{3}{2} \left( r'_{\beta}\mu_{\alpha} + r'_{\alpha}\mu_{\beta} \right) + \left( \sum_{\alpha} r'_{\alpha}\mu_{\alpha} \right) \delta_{\alpha\beta}. \end{aligned}$$

631 Table 8.7.3.2, replace entries in third column by

$$V_T j_0(2\pi h_x \delta_x) j_0(2\pi h_y \delta_y) j_0(2\pi h_z \delta_z)$$

for  $\hat{\gamma} = 1$ ,

$$egin{aligned} -i V_T \, \delta_lpha \, j_1(2\pi h_lpha \, \delta_lpha) \ & imes \, j_0(2\pi h_eta \, \delta_eta) j_0(2\pi h_\gamma \, \delta_\gamma) \end{aligned}$$

for  $\hat{\gamma} = r_{\alpha}$ ,

$$egin{aligned} &-V_T\delta_lpha\delta_eta j_1(2\pi h_lpha\delta_lpha)\ & imes j_1(2\pi h_eta\delta_eta) j_0(2\pi h_\gamma\delta_\gamma) \end{aligned}$$

for  $\hat{\gamma} = r_{\alpha}r_{\beta}$ .

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

$$\nabla E_{11} = +(3/5) \big( \pi P_{22+} - 3^{1/2} P_{20} \big) Q_r$$
  
$$\nabla E_{22} = -(3/5) \big( \pi P_{22+} + 3^{1/2} P_{20} \big) Q_r.$$

Equation following equation (8.7.3.33), replace "R(r)r" with "[R(r)/r]".

Equation (8.7.3.34), change " $\frac{1}{2}$ " to " $\frac{1}{3}$ ". Left column, line 1, change " $V_{\alpha\beta}$ " to " $Q_{\alpha\beta}$ ". 632 Left column, line 23, replace "for the electronic charge distribution" with "for a charge distribution". Equation (8.7.3.39*a*), change " $V^2$ " to "V". Right column, line 11, change "may" to "must". Equation (8.7.3.39b), change " $V^2$ " to "V".

- Table 8.7.3.5, footnote \*, replace " $e'_{q-} = \sqrt{(2/3)}d_{yz}$ " 634 with " $e'_{g-} = \sqrt{(1/3)}d_{xz} - \sqrt{(2/3)}d_{yz}$ " Equation (8.8.3*a*), change " $s^2$ " to " $s_g^2$ ".
- 646
- 649 References to Section 8.2, line 1, change "WELCH" to "WELSCH".
- 650 References to Section 8.5, line 6, change "WELCH" to "WELSCH".

- References for Section 8.7, change "COPPENS, P. (1992)" to "COPPENS, P. (1993)".
   References for Section 8.7, change "International Tables for Crystallography (1992)" to "International Tables for Crystallography (1993)".
- 659 Replace "Note added in proof" with "Addendum" Replace Addendum to 9.1.1.3 with

"9.1.1.3. Full details of tetragonal sphere packings have now been published by W. Fischer [Tetragonal sphere packings. I. Lattice complexes with zero or one degree of freedom. (1991). Z. Kristallogr. 194, 67–85; II. Lattice complexes with two degrees of freedom. (1991). Z. Kristallogr. 194, 87–110; III. Lattice complexes with three degrees of freedom. (1993). Z. Kristallogr. 205, 9–26].

A paper by M. O'Keeffe [Dense and rare fourconnected nets. (1991). Z. Kristallogr. 196, 21-37] gives new results for dense and rare packings. M. O'Keeffe & N. E. Brese [Uninodal 4-connected 3D nets. I. Nets without 3- or 4-rings. (1992). Acta Cryst. A48, 663-669] and M. O'Keeffe [Uninodal 4-connected 3D nets. II. Nets with 3-rings. (1992). Acta Cryst. A48, 670-673] have studied 4-connected nets which have symmetrically equivalent nodes, edges of equal length, and no shorter distances between nodes. Their 43 such nets therefore correspond uniquely to 43 types of homogeneous sphere packings."

Replace Addendum to 9.1.2 with

"9.1.2. M. Tanemura & T. Matsumoto [On the density of the p31m packing of ellipses. (1992). Z. Kristallogr. **198**, 88–99] give new results for the packing of ellipses."

- 671 Right column, line 12, remove comma after "conditions".
- 673 Right column, line -17, change "Subsection" to "§". Right column, footnote, change "AlOH)<sub>3</sub>" to "Al(OH)<sub>3</sub>".
- 674 Left column, line -22, change "the USSR" to "the former USSR".
- 678 Fig. 9.2.2.16, replace the following labels: "24" below  $\bar{26}$  with "2 $\bar{4}$ ", "33" below  $0\bar{6}$  with "3 $\bar{3}$ ", "33" below 06 with " $\bar{3}$ 3", "45" below 19 with " $\bar{45}$ ", "21" below 26 with " $\bar{24}$ ", "36" below 39 with " $\bar{36}$ ". Right column, line -3, change "2/m" to "21/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."
- Right column, line 3, missing symbol should be "x<sub>i</sub>".
   Right column, line 32, replace "two (P3 and R3) of the four" with "three (P1, P3, R3) of the five".
- 796 Right column, add after Note:

"Addendum

Further papers, in which the effect of molecular symmetry and of degree of symmorphism are discussed,

have appeared since the first printing of this Volume [A. J. C. Wilson (1991). Space groups rare for organic structures: the arithmetic crystal class mmmP. Z. Kristallogr. 197, 85–88; (1992). Popularity: holiday musings on space groups. BCA Crystallography News, No. 41, p. 20; (1993). Space groups rare for organic structures. III. Symmorphism and inherent molecular symmetry. Acta Cryst. A49, 795–806. The proportion of structures in which molecules make use of their inherent symmetry is greater than Wilson (1988) supposed."

- 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 "Féderation" to "Fédération".
- 852 Table 10.3.1 (cont.), Germany, Federal Republic of entry, change "Verordinung" 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 Sante 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 "Parrett, 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 "9.2.2" for "Schrauber, H."; delete "Schuttke, G.H., 5.3"; add "5.3" to
  "Schwuttke, G.H.".
- 863 Add "Skov Pedersen, J.; see Pedersen, J.S."; add "6.1.1" to "Smith, V.H."; add "Thakkar, A.J., 6.1.1"; change "Theussen, G." to "Thuesen, G.".
- 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"; add "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"; add "Symmorphism, 796".