

## International Tables Volume C

### Timetable

- (1) Editor to contact as many authors of existing chapters as possible by end of July 2009.
- (2) Editorial Office to try to contact remaining authors by end of August 2009.
- (3) Revisions of existing chapters to be sent to Editor by October 2009.
- (4) Authors of new articles to send Editor an outline by end of September 2009 with full article to be submitted by end of February 2010.
- (5) New articles to be peer reviewed March-July 2010.
- (6) New articles to be sent to Editorial Office by August 2010.
- (7) Volume to go to press by August 2011.

### New articles

*In situ* preparation of crystals (low temperature) - Roland Boerse?

High-throughput studies - Chris Gilmore?

Article on extinction corrections (H.-C. Hu) - to be discussed with Pierre Becker. Article is too long at present?

Joke Hadermann has sent suggestions for revisions for articles on electron crystallography.

### Existing articles

| Part/Chapter  | Section | Present authors               | Authors for next edition | Comments   |
|---|---------|-------------------------------|--------------------------|--|
| Part 1. Crystal geometry and symmetry                       |         |                               |                          |  |
| 1.1. Summary of general formulae                            |         | E. Koch                       | E. Koch                  | Editor to ask whether revision needed. If not, keep as is.                             |
| 1.2. Application to the crystal systems                     |         |                               |                          |  |
| 1.3. Twinning   |         |                               |                          |  |
| 1.4. Arithmetic crystal classes and symmorphic space groups |         | A. J. C. Wilson               |                          | Editor to ask Mois Aroyo to check this article is still up to date <i>cf.</i> Volume A |
| Part 2. Diffraction geometry and its practical realization  |         |                               |                          |  |
| 2.1. Classification of experimental techniques              |         | J. Helliwell                  | J. Helliwell             | REVISIONS RECEIVED   |
| 2.2. Single-crystal X-ray techniques                        |         |                               |                          |  |
| 2.3. Powder and related techniques: X-ray techniques        |         | W. Parrish and J. I. Langford |                          | Langford contacted - does not want to update. Editor might update this article.        |

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| 2.4. Powder and related techniques: electron and neutron techniques | 2.4.1. Electron techniques                               | J. M. Cowley  |  | Editor might update these articles                                  |
|   | 2.4.2. Neutron techniques                                | A. W. Hewat   |  |   |
| 2.5. Energy-dispersive techniques                                   | 2.5.1. Techniques for X-rays                             | B. Buras and L. Gerward                             |  | REVISION RECEIVED   |
|   | 2.5.2. White-beam and time-of-flight neutron diffraction | J. D. Jorgensen, W. I. F. David and B. T. M. Willis |  | No reply from David. Editor will discuss this article with Lander   |
| 2.6. Small-angle techniques   | 2.6.1. X-ray techniques                                  | O. Glatter  |  | Glatter unable to update - include this article as it is at present |
|   | 2.6.2. Neutron techniques                                | R. May  |  | May has agreed to update  |
| 2.7. Topography   |  | A. R. Lang  |  | Lang unable to update - leave this article as it is at present      |
| 2.8. Neutron diffraction topography                                 |  | M. Schlenker and J. Baruchel                        |  | Schlenker will update   |
| 2.9. Neutron reflectometry  |  | G. S. Smith and C. F. Majkrzak                      |  | Authors contacted? Leave this article as it is at present           |
| <b>Part 3. Preparation and examination of specimens</b>             |  |   |  |   |
| 3.1. Preparation, selection, and investigation of specimens         |  | P. F. Lindley                                       |  | Lindley unable to update - leave this article out of new edition?   |
| 3.2. Determination of the density of solids                         | 3.2.1. Introduction                                      | P. F. Lindley                                       |  | Leave these articles as they are at present                         |
|   | 3.2.2. Description and discussion of techniques          | F. M. Richards                                      |  |   |
|   | 3.2.3. Biological macromolecules                         | P. F. Lindley                                       |  |   |
| 3.3. Measurement of refractive index                                |  | E. S. Larsen Jr, R. Meyrowitz and A.                |  | Bohaty to rewrite with Petra Becker                                 |

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|  |  | J. C. Wilson   |  |   |
| 3.4. Mounting and setting of specimens for X-ray crystallographic studies      |  | P. F. Lindley  |  | Lindley unable to update. This article is now out of date - leave out of new edition?                               |
| 3.5. Preparation of specimens for electron diffraction and electron microscopy |  | N. J. Tighe, J. R. Fryer and H. M. Flower                        |  | Authors say this would be a long article if rewritten. Find a new author or leave this article as it is at present. |
| 3.6. Specimens for neutron diffraction   |  | B. T. M. Willis  |  | Not needed - leave this article out of new edition.   |
| Part 4. Production and properties of radiations                                |  |  |  |   |
| 4.1. Radiations used in crystallography  |  | V. Valvoda   |  | Rafaja will rewrite this  |
| 4.2. X-rays  | 4.2.1. Generation of X-rays  | U. W. Arndt  |  | Leave these articles as they are at present   |
|  | 4.2.2. X-ray wavelengths   | R. D. Deslattes, E. G. Kessler Jr, P. Indelicato and E. Lindroth |  |   |
|  | 4.2.3. X-ray absorption spectra  | D. C. Creagh   |  | Creagh will revise  |
|  | 4.2.4. X-ray absorption (or attenuation) coefficients                            | D. C. Creagh and J. H. Hubbell                                   |  |   |
|  | 4.2.5. Filters and monochromators  | D. C. Creagh   |  |   |
|  | 4.2.6. X-ray dispersion corrections  | D. C. Creagh   |  |   |
| 4.3. Electron diffraction  | 4.3.1. Scattering factors for the diffraction of electrons by crystalline solids | J. M. Cowley   |  | Colliex and Spence will update. Form-factor tables to be available only online (not in print); formula and a few    |

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|                         |  |  |  | examples will be given in print.  |
|                         | 4.3.2. Parameterizations of electron atomic scattering factors   | J. M. Cowley, L. M. Peng, G. Ren, S. L. Dudarev and M. J. Whelan |  |   |
|                         | 4.3.3. Complex scattering factors for the diffraction of electrons by gases                            | A. W. Ross, M. Fink, R. Hilderbrandt, J. Wang and V. H. Smith Jr |  |   |
|                         | 4.3.4. Electron energy-loss spectroscopy on solids   | C. Colliex   |  |   |
|                         | 4.3.5. Oriented texture patterns   | B. B. Zvyagin  |  |   |
|                         | 4.3.6. Computation of dynamical wave amplitudes  | D. F. Lynch and A. Howie   |  |   |
|                         | 4.3.7. Measurement of structure factors and determination of crystal thickness by electron diffraction | J. Gjønnes and J. W. Steeds                                      |  |   |
|                         | 4.3.8. Crystal structure determination by high-resolution electron microscopy                          | J. C. H. Spence and J. M. Cowley                                 |  |   |
| 4.4. Neutron techniques | 4.4.1. Production of neutrons  | J. M. Carpenter and G. Lander                                    |  | REVISION RECEIVED for 4.4.1. Lander will also update the rest of the chapter. Keep scattering lengths for neutrons, magnetic form factors and absorption coefficients for neutrons in printed volume. Editor to |

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|  |  |  |  | check numbers in these tables are up to date.   |
|  | 4.4.2. Beam-definition devices                                       | I. S. Anderson and O. Schärpf                  |  |   |
|  | 4.4.3. Resolution functions  | R. Pynn and J. M. Rowe                         |  |   |
|  | 4.4.4. Scattering lengths for neutrons                               | V. F. Sears                                    |  |   |
|  | 4.4.5. Magnetic form factors   | P. J. Brown                                    |  |   |
|  | 4.4.6. Absorption coefficients for neutrons                          | B. T. M. Willis                                |  |   |
| Part 5. Determination of lattice parameters      |  |  |  |   |
| 5.1. Introduction                                |  | A. J. C. Wilson                                |  | Editor unsure what to do with this part - will discuss with Robert Dinnebier. None of the present authors available to update articles. Might combine this part with a chapter on powder diffraction. |
| 5.2. X-ray diffraction methods: polycrystalline  |  | W. Parrish, A. J. C. Wilson and J. I. Langford |  |   |
| 5.3. X-ray diffraction methods: single crystal   |  | E. Galdecka                                    |  |   |
| 5.4. Electron-diffraction methods                | 5.4.1. Determination of cell parameters from single-crystal patterns | A. W. S. Johnson                               |  |   |
|  | 5.4.2. Kikuchi and HOLZ techniques                                   | A. Olsen                                       |  |   |
| 5.5. Neutron methods                             |  | B. T. M. Willis                                |  |   |
| Part 6. Interpretation of diffracted intensities |  |  |  |   |

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| 6.1. Intensity of diffracted intensities     | 6.1.1. X-ray scattering                        | E. N. Maslen, A. G. Fox and M. A. O'Keefe |  | Form-factor tables to be available only online (not in print). Otherwise leave this part as it is at present. |
|  | 6.1.2. Magnetic scattering of neutrons         | P. J. Brown                               |  |   |
|  | 6.1.3. Nuclear scattering of neutrons          | B. T. M. Willis                           |  |   |
| 6.2. Trigonometric intensity factors         |  | H. Lipson, J. I. Langford and H.-C. Hu    |  |   |
| 6.3. X-ray absorption                        |  | E. N. Maslen                              |  |   |
| 6.4. The flow of radiation in a real crystal |  | T. M. Sabine                              |  |   |
| Part 7. Measurement of intensities           |  |   |  |   |
| 7.1. Detectors for X-rays                    | 7.1.1. Photographic film                       | P. M. de Wolff                            |  | REVISION RECEIVED for 7.1.5. New author (ESRF beamline scientist, Amemiya?) to update remainder?              |
|  | 7.1.2. Geiger counters                         | W. Parrish and J. I. Langford             |  |   |
|  | 7.1.3. Proportional counters                   | W. Parrish and J. I. Langford             |  |   |
|  | 7.1.4. Scintillation and solid-state detectors | W. Parrish and J. I. Langford             |  |   |
|  | 7.1.5. Energy-dispersive detectors             | B. Buras and L. Gerward                   |  |   |
|  | 7.1.6. Position-sensitive detectors            | U. W. Arndt                               |  |   |
|  | 7.1.7. X-ray-sensitive TV cameras              | J. Chikawa                                |  |   |
|  | 7.1.8. Storage phosphors                       | Y. Amemiya and J. Chikawa                 |  |   |
| 7.2. Detectors for                           |  | J. N. Chapman                             |  | Colliex to update   |

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| electrons  |  |   |  |   |
| 7.3. Thermal neutron detection   |  | P. Convert and P. Chieux  |  | Editor to update                            |
| 7.4. Correction of systematic errors                                   | 7.4.1. Absorption                                      | N. G. Alexandropoulos, M. J. Cooper, P. Suortti and B. T. M. Willis |  | Leave this chapter as it is at present      |
|  | 7.4.2. Thermal diffuse scattering                      | B. T. M. Willis   |  |   |
|  | 7.4.3. Compton scattering                              | N. G. Alexandropoulos and M. J. Cooper                              |  |   |
|  | 7.4.4. White radiation and other sources of background | P. Suortti  |  |   |
| 7.5. Statistical fluctuations  |  | A. J. C. Wilson   |  | Leave this chapter as it is at present      |
| Part 8. Refinement of structural parameters                            |  |   |  |   |
| 8.1. Least squares   |  | E. Prince and P. T. Boggs   |  | Leave these chapters as they are at present |
| 8.2. Other refinement methods  |  | E. Prince and D. M. Collins   |  |   |
| 8.3. Constraints and restraints in refinement                          |  | E. Prince, L. W. Finger and J. H. Konnert                           |  |   |
| 8.4. Statistical significance tests                                    |  | E. Prince and C. H. Spiegelman                                      |  |   |
| 8.5. Detection and treatment of systematic error                       |  | E. Prince and C. H. Spiegelman                                      |  |   |
| 8.6. The Rietveld method   |  | A. Albinati and B. T. M. Willis                                     |  | Albinati might revise                       |
| 8.7. Analysis of charge and spin densities                             |  | P. Coppens, Z. Su and P. J. Becker                                  |  | Becker will revise                          |
| 8.8. Accurate structure-factor determination with electron diffraction |  | J. Gjønnnes   |  | No reply from Gjønnnes - ask Hoffmøller?    |
| Part 9. Basic structural features                                      |  |   |  |   |

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| 9.1. Sphere packings and packings of ellipsoids  |   | E. Koch and W. Fischer   |  | REVISION RECEIVED                      |
| 9.2. Layer stacking  | 9.2.1. Layer stacking in close-packed structures      | D. Pandey and P. Krishna   |  | No reply from Pandey                   |
|  | 9.2.2. Layer stacking in general polytypic structures | S. Āuroviĉ   |  | Āuroviĉ unable to update               |
| 9.3. Typical interatomic distances: metals and alloys  |   | J. L. C. Daams, J. R. Rodgers and P. Villars                     |  | Any reply from authors?                |
| 9.4. Typical interatomic distances: inorganic compounds  |   | G. Bergerhoff and K. Brandenburg                                 |  | Bergerhoff will revise if required     |
| 9.5. Typical interatomic distances: organic compounds  |   | F. H. Allen, D. G. Watson, L. Brammer, A. G. Orpen and R. Taylor |  | Leave this chapter as it is at present |
| 9.6. Typical interatomic distances: organometallic compounds and coordination complexes of the d - and f -block metals |   | A. G. Orpen, L. Brammer, F. H. Allen, D. G. Watson and R. Taylor |  | Leave this chapter as it is at present |
| 9.7. The space-group distribution of molecular organic structures  |   | A. J. C. Wilson, V. L. Karen and A. Mighell                      |  | Response from Karen?                   |
| 9.8. Incommensurate and commensurate modulated structures  |   | T. Janssen, A. Janner, A. Looijenga-Vos and P. M. de Wolff       |  | REVISION RECEIVED                      |
| Part 10. Precautions against radiation injury  |   |  |  |  |
| 10.1. Introduction   |   | D. C. Creagh and S. Martinez-Carrera                             |  | Creagh will revise                     |

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| 10.2. Protection from ionizing radiation |  |  |  |  |
| 10.3. Responsible bodies                 |  |  |  |  |