

## International Union of Crystallography

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### International Tables for Crystallography Volume B: Reciprocal Space

Edited by U. Shmueli

Reprinted with corrections and additions 1996

#### Corrigenda and Addenda to the First Edition (1993)

A corrected reprint of *International Tables for Crystallography* Volume B was published in February 1996. Corrections and additions to the First Edition are listed below.

*Page*

- 13 Table 1.2.7.1, for  $l = 3$ , change entry in fourth column to

$$\left. \begin{array}{l} 5z^2 - 3z \\ x[5z^2 - 1] \\ y[5z^2 - 1] \\ (x^2 - y^2)z \\ 2xyz \\ x^3 - 3xy^2 \\ -y^3 + 3x^2y \end{array} \right\}$$

Table 1.2.7.1, last column, entry for 66+, change “0.54688” to “0.54687”.

- 14 Table 1.2.7.1. (*cont.*), last column, entry for 71+, change “0.6488” to “0.06488”.

Table 1.2.7.1. (*cont.*), change entry in fourth column for  $l = 7$ , symbol 71 – to

$$(429z^6 - 495z^4 + 135z^2 - 5)y$$

Table 1.2.7.1. (*cont.*), replace footnotes \* and † with

\* Common factor such that  $Cc_{imp} = P_l^m(\cos \theta) \frac{\cos m\varphi}{\sin m\varphi}$ .

†  $N_{\text{ang}} = \{(14A_+^5 - 14A_-^5 - 20A_+^3 + 20A_-^3 + 6A_+ - 6A_-)2\pi\}^{-1}$  where:  $A_{\pm} = [(30 + \sqrt{480})/70]^{1/2}$ .

- 16 Table 1.2.7.4, add “Su & Coppens, 1990” to end of table heading.
- 122 Table B.6, entry 88  $I4_1/a$  (Origin 1), change “–I” to “I” in last column.
- 123 Table B.6. (*cont.*), entry 129  $P4/nmm$  (Origin 1), change entry in last column to “P –4 –2 –1AB”; entry 130  $P4/ncc$  (Origin 1), change entry in last column to “P –4 2N –1AB”.
- 124 Table B.6. (*cont.*), entry 153, change “(0 0 –2)” to “(0 0 2)” in last column.
- 189 Equation (2.1.5.10), change “ $^{-1/2}$ ” to “ $^{1/2}$ ”.
- Equation (2.1.5.11), change “ $^{-1/2}$ ” to “ $^{1/2}$ ”.
- 242 Equation (2.3.4.1), replace “ $x$ ” with “ $x_j$ ” in both exponentials.
- Line 19, replace “ $F_h^2$ ” with “ $|F_h|^2$ ”.
- Line 21, replace “ $F_h^2$ ” with “ $|F_h|^2$ ”.
- Line –3, replace “ $\sum_{j,k}$ ” with “ $\sum_{ij}$ ”.
283. Equation (2.5.1.7), replace “ $\psi(\mathbf{r}')\psi(\mathbf{r}') d\mathbf{r}'$ ” with “ $\varphi(\mathbf{r}')\psi(\mathbf{r}') d\mathbf{r}'$ ”.

- 289 Line 32, change “(2.5.1.48)” to “(2.5.1.49)”.

Line 43, change “(2.5.1.44)” to “(2.5.1.43)”.

- 385 Left column, line 37, replace equation with

$$T = \frac{1}{2} \sum_{\kappa l \alpha} m(\kappa) \dot{u}_\alpha^2(\kappa l)$$

Right column, equation (4.1.2.1), replace first line of equation with

$$H = \frac{1}{2} \sum_{\kappa l \alpha} m(\kappa) \dot{u}_\alpha^2(\kappa l)$$

- 387 Equation (4.1.3.6), replace “ $|G_j(\mathbf{Q}, \mathbf{q})|^2$ ” with “ $|G_j(\mathbf{Q}, \mathbf{q})|^2$ ”.

- 465 Equation (5.1.2.6), replace “ $\sum$ ” with “ $\sum_j$ ”.

Equations (5.1.2.8), (5.1.2.14) and (5.1.2.15), replace “ $\sum$ ” with “ $\sum_h$ ”.

- 466 Left column, line 17, change “this number” to “their number”.

Right column, line 24, change “to the zero” to “to zero”.

- 467 Fig. 5.1.2.5 caption, change “for two states” to “for the two states”.

- 468 Left column, line 26, change “Fig. 5.3.2.b” to “Fig. 5.1.3.2b”.

- 469 Equation (5.1.3.6), replace with

$$\delta = R\lambda^2 |C| \sqrt{|\gamma| F_h F_{\bar{h}}} / [\pi V \sin 2\theta]$$

- 470 Left column, line 37, change “let  $I_{01}, I_{h1}$ ” to “let  $I_{01}, I_{02}$ ”.

Left column, line 39, change “ $\overline{I_{01}I_{h1}}$  and  $\overline{I_{02}I_{h2}}$ ” to “ $\overline{I_{01}I_{h2}}$  and  $\overline{I_{02}I_{h1}}$ ”.

Equation (5.1.3.12), replace first equation with

$$A_L = 1/\overline{A_2 A_1}$$

Right column, line 1, change “ $T_0$  and  $T_h$ ” to “ $T_0, T_h$  and  $T_0'$ ”.

Right column, lines 5 and 6, change “The tie points  $A_1$  and  $A_2$  correspond to  $\eta = 1$  and  $\eta = -1$ ” to “The tie points  $I_1$  and  $I_2$  correspond to  $\eta = -1$  and  $\eta = +1$ ”.

Right column, line 9, change “ $\overline{I_{01}I_{02}/k}$ ” to “ $\overline{I_{01}I_{02}/k}$ ”.

Right column, line 10, change “ $\overline{O_{01}I_{h1}}$ ” to “ $\overline{I_{01}I_{h1}}$ ”.

- 473 Left column, line 25, change “ $2\pi\Lambda^{-1}$ ” to “ $2\pi t\Lambda^{-1}$ ”.

Left column, line 27, add “ $t$ ” after  $j$ .

Left column, line 28, change “ $\cos(2\pi\Lambda^{-1})$ ” to “ $\cos(2\pi t\Lambda^{-1})$ ”.

- 474 Left column, line –9, change “ $J_0^{-1}(z)$ ” to “ $J_0(z)$ ”.

Left column, line –7, change “ $\mu t$ ” to “ $\mu_0 t$ ”.

Right column, line 5, replace with

$$f_1(\eta) = \left[ \frac{\sin U\eta}{U\eta} \right]^2$$

- 475 Left column, line 10, change “maximum” to “minimum”.

Fig. 5.1.7.3 caption, insert space after “Variation”.

- 476 Left column, line 4, change " $\mathbf{D}_h^{(d)}$ " to " $\mathbf{D}_0^{(d)}$ ".  
 Right column, line 13, change " $\sqrt{K^2 \Lambda_B^2 + 1}$ " to " $\sqrt{K^2 \Lambda_B^2 t^2 + 1}$ ".
- 477 Left column, line 3, replace with  

$$[\sin(\pi t \eta / \Lambda_B) / \eta]^2$$

- 477 Left column, line 6, change the first denominator to " $V^2 \sin^2 \theta$ " and the second denominator to " $2\pi k \cos \theta r \Delta \theta$ ".  
 Left column, line 29, change "expansion" to "extension".
- 479 Right column, line 14, replace " $\mathbf{B}_{N1} - \mathbf{D}_{N2} = 0$ " with  
 $\mathbf{B}_{N1} - \mathbf{B}_{N2} = 0$ .

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## International Union of Crystallography Keywords for the World Database of Crystallographers

*Y. Epelboin, General Editor, LMCP, Université P. M. Curie, URA009, CNRS, case 115, 75252 Paris CEDEX 05, France. E-mail: epelboin@lmcp.jussieu.fr*

The *World Database of Crystallographers*, installed in Chester (URL: <http://www.iucr.ac.uk/>) is now being updated.

Selection by means of keywords is one of the most powerful methods of rapidly retrieving useful names. In the previous edition, the keywords list was sorted in three parts: *Methods, Properties and Applications, Compounds and Attributes* [*Acta Cryst.* (1992), **A48**, 949–954]. It contained about 1500 keywords.

This new edition contains 2000 keywords. They have been selected using the 9th edition of the *World Directory*. Words never or seldom used have been removed (about 300), and new ones taken from the field 'other interests', where scientists could use their own wording, have been added. Thus, all communities should be able to describe their interests properly. Acronyms have been carefully checked and retained when in agreement with real use. The singular has been used everywhere.

Separation into three different sublists has been suppressed. In the previous edition, scientists mixed words from the three lists to create their own keywords and so this distinction proved useless.

Note that the phrase 'X-ray\_diffraction', which uses two words joined by an underscore character, will be treated as one keyword, whereas the phrase 'X-ray diffraction' represents two keywords. The meaning is different. The first case represents all techniques which use X-ray diffraction. The second case refers to all techniques which use X-rays (including non-diffraction techniques) and all diffraction techniques involving other particles such as neutrons or electrons.

The International Union of Crystallography has been one of the first Unions to provide such a service to the Community. The number of daily interrogations of the database has proved the need for such a service. I hope that a better definition of the keywords will help in improving this service.

1D	Adamantane	Algorithm	Amphiphilic	Anti
2D	Addiction	Alignment	Amylase	Antiallergic
3D	Additive	Aliphatic	Amyrin	Antibacterial
4D	Adenovirus	Alkali	Anaemia	Antibiotic
5D	Adhesion	Alkaline	Analgesic	Antibody
II-VI	Adsorbate	Alkaloid	Analysis	Anticancer
II-VII	Adsorption	Alkane	Analytical	Anticoagulant
III-V	Advanced	Alkoxide	Analyzer	Antidepressant
IV-VI	AEM	Allotropy	Anatomy	Antiestrogen
Aberation	Aerodynamics	Allotropy	Angiogenesis	Antiferroelectricity
Ablation	Aerosol	Alloy	Angle	Antiferromagnetism
Absolute	Aerospace	Alteration	Anharmonic	Antifolate
Absorption	AES	Alumina	Anharmonicity	Antigen
Accuracy	Affinity	Aluminate	Anhydase	Antimalarial
Accurate	AFM	Aluminium	Anhydrolase	Antimicrobial
Acetylene	Agent	Aluminophosphate	Anhydrous	Antimony
Acid	Aggregate	Aluminosilicate	Animal	Antimiscarinic
Acidophile	Agonist	Alzheimer's	Animation	Antiphase
Acoustics	Agrochemistry	Americium	Anion	Antitumor
Acoustooptics	Aided	Amide	Anisotropic	Antiulcer
Actin	AIDS	Amidotransferase	Anisotropy	Antiviral
Actinide	Air	Amino	Annealing	Anvil
Activation	Alanine	Aminotransferase	Annexin	Apatite
Active	Albumin	Amorphization	Annihilation	Aperiodic
Activity	Alcohol	Amorphous	Anomalous	Apparatus
Actuator	Aldolase	Amphibole	Anomaly	Application