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Hydrogen bonding and thermal vibrations in crystalline phosphate salts of histidine and imidazole. Erratum.

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Abstract

In Blessing [*Acta Cryst.* (1986), B42, 613-621] a mistake was made in converting from the least-squares refined b_{ij} values to the reported U_{ij} values. The cross-term U_{ij} values, $i \neq j$, and their e.s.d.'s should be doubled.

The thermal-ellipsoid drawings and the reported riding model corrections to the P–O bond lengths were based on the b_{ij} values and are correct, but the rigid-bond and rigid-molecule tests and the rigid-body **TLS** analyses were based on the incorrect U_{ij} values. New analyses using the corrected U_{ij}'s gave considerably improved rigid-group test results and statistics of fit for the **TLS** models, but the rigid-body libration corrections to the P–O bond lengths did not change very much.* The new corrections are, on average, 0·002 Å larger than the old ones, and they are generally closer to the riding model corrections. It now appears that the refined thermal parameters are more accurate than they were thought to be, and it no longer seems clear that the rigid-body model is inferior to the riding model for the phosphate groups. The author apologizes for his error.

* Lists of corrected *U*, *T*, *L* and *S* values, rigid-group test results, and libration corrected P–O bond lengths have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43973 (15 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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The Ewald Prize

The first Ewald Prize for outstanding contributions to the science of crystallography has been awarded jointly to Professor **J. M. Cowley** and Dr **A. F. Moodie**, for their outstanding achievements in electron diffraction and microscopy, especially for their fundamental contributions to the theory and technique of direct imaging of crystal structures and structure defects by high-resolution electron microscopy.

Their pioneering work on the dynamical scattering of electrons was reported in a series of papers in *Acta Crystallographica* and other journals from 1957 onwards. A theory of Fourier images led them to the multi-slice formulation of the scattering of an electron wave in its passage through a crystal. This formulation is able to take into account many hundreds of scattered beams, and has become the basis of widely used computer programs. The theory allows electron micrographs, obtained with modern high-resolution instruments, to be reliably and quantitatively interpreted, and used for the determination of the structures of both perfect crystals and crystals containing defects.

Professor Cowley and Dr Moodie, together and separately, have made many further contributions to theory, methods and results in electron diffraction and microscopy. Their work has often stressed a unified approach to diffraction and microscopy through physical optics. An overview of the whole field may be found in Professor Cowley's book *Diffraction Physics* [(1981). Amsterdam: North-Holland].

John Maxwell Cowley, born in Australia in 1923 and a graduate of Adelaide University, was formerly a Chief Research Scientist at the Division of Chemical Physics, CSIRO, Melbourne, Australia. Later he was Professor of Physics at the University of Melbourne, and since 1970 has been the Galvin Professor of Physics at Arizona State University, Tempe, USA.

Alexander Forbes Moodie, born in Scotland in 1923, graduated from St Andrews University in 1948. Since then he has been a member of CSIRO in Australia where he is a Chief Research Scientist at the Divison of Chemical Physics. This Division was incorporated into the Division of Materials Science and Technology at the end of 1986.

The presentation of the Ewald Prize, which consists of a medal and a certificate for each awardee and a shared award of US $20 000, will take place at the Opening Ceremony of the XIV International Congress of Crystallography at Perth, Western Australia, on 12 August 1987. An honorary medal will be presented to the Ewald family during the ceremony.

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