densities (see *e.g.* Smith *et al.*, 1977). A number of examples of displacement deformation densities of high symmetry are shown in Fig. 1.9.4.1 as three-dimensional contour maps.

1.9.5. Glossary

$b^{ijk\ldots}$	atomic displacement tensor
β^{ij}, $U^{ijk\ldots}$	atomic displacement parameter
g_{ij}	metric tensor
S_α	atomic static Debye–Waller factor
T_α	atomic thermal Debye–Waller factor
$\mathbf{Q}$	scattering vector
u^i	atomic displacement

References

Hazell, R. G. & Willis, B. T. M. (1978). *Correlations between third cumulants in the refinement of noncentrosymmetric structures. Acta Cryst.* A**34**, 809–811.

Hummel, W., Raselli, A. & Bürgi, H.-B. (1990). *Analysis of atomic displacement parameters and molecular motion in crystals. Acta Cryst.* B**46**, 683–692.

International Tables for Crystallography (1999). Vol. C. *Mathematical, physical and chemical tables*, edited by A. J. C. Wilson & E. Prince. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (2001). Vol. B. *Reciprocal space*, edited by U. Shmueli. Dordrecht: Kluwer Academic Publishers.

International Tables for Crystallography (2002). Vol. A. *Space-group symmetry*, edited by Th. Hahn. Dordrecht: Kluwer Academic Publishers.

Jahn, H. A. (1949). *Note on the Bhagavantam–Suryanarayana method of enumerating the physical constants of crystals. Acta Cryst.* **2**, 30–33.

Johnson, C. K. (1965). *ORTEP – a FORTRAN thermal ellipsoid plot program.* Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

Johnson, C. K. (1970). *Generalized treatments for thermal motion*. In *Thermal neutron diffraction*, edited by B. T. M. Willis, pp. 132–160. Oxford University Press.

Kuhs, W. F. (1983). *Statistical description of multimodal atomic probability densities. Acta Cryst.* A**39**, 148–158.

Kuhs, W. F. (1984). *Site-symmetry restrictions on thermal-motion-tensor coefficients up to rank 8. Acta Cryst.* A**40**, 133–137.

Kuhs, W. F. (1988). *The anharmonic temperature factor in crystallographic structure analysis. Aust. J. Phys.* **41**, 369–382.

Kuhs, W. F. (1992) *Generalized atomic displacements in crystallographic structure analysis. Acta Cryst.* A**48**, 80–98.

Kuznetsov, P. I., Stratonovich, R. L. & Tikhonov, V. I. (1960). *Quasi-moment functions in the theory of random processes. Theory Probab. Its Appl. (USSR)*, **5**, 80–97.

Levy, H. A. (1956). *Symmetry relations among coefficients of the anisotropic temperature factor. Acta Cryst.* **9**, 679.

Nelmes, R. J. (1969). *Representational surfaces for thermal motion. Acta Cryst.* A**25**, 523–526.

Pach, K. & Frey, T. (1964). *Vector and tensor analysis*. Budapest: Terra.

Peterse, W. J. A. M. & Palm, J. H. (1966). *The anisotropic temperature factor of atoms in special positions. Acta Cryst.* **20**, 147–150.

Scheringer, C. (1985). *A deficiency of the cumulant expansion of the anharmonic temperature factor. Acta Cryst.* A**41**, 79–81.

Sirotin, Yu. I. (1960). *Group tensor spaces. Sov. Phys. Crystallogr.* **5**, 157–165.

Sirotin, Yu. I. (1961). *Plotting tensors of a given symmetry. Sov. Phys. Crystallogr.* **6**, 263–271.

Smith, V. H. Jr, Price, P. F. & Absar, I. (1977). *Representations of electron density and its topographical features. Isr. J. Chem.* **16**, 187–197.

Trueblood, K. N., Bürgi, H.-B., Burzlaff, H., Dunitz, J. D., Gramaccioli, C. M., Schulz, H. H., Shmueli, U. & Abrahams, S. C. (1996). *Atomic displacement parameter nomenclature. Report of a subcommittee on atomic displacement parameter nomenclature. Acta Cryst.* A**52**, 770–781.

Willis, B. T. M. & Pryor, A. W. (1975). *Thermal vibrations in crystallography*. Cambridge University Press.

Wondratschek, H. (1958). *Über die Möglichkeit der Beschreibung kristallphysikalischer Eigenschaften durch Flächen. Z. Kristallogr.* **110**, 127–135.

Zucker, U. H. & Schulz, H. (1982*a*). *Statistical approaches for the treatment of anharmonic thermal motion in crystals. I. A comparison of the most frequently used formalisms of anharmonic thermal vibrations. Acta Cryst.* A**38**, 563–568.

Zucker, U. H. & Schulz, H. (1982*b*). *Statistical approaches for the treatment of anharmonic thermal motion in crystals. II. Anharmonic thermal vibrations and effective atomic potentials in the fast ionic conductor lithium nitride Li_3N. Acta Cryst.* A**38**, 568–576.