

inorganic compounds, such as most minerals.

Besides confirming the physical meaning of ADPs, a detailed interpretation of atomic motion is allowed, also in terms of internal degrees of freedom of atomic groups and their correlated motion. The possibility of correcting bond lengths for thermal motion in the most general case is also provided, since the correlation tensors between the displacement of different atoms can be obtained as by-products; particularly interesting is the link to spectroscopic and thermodynamic properties, and the possibility of checking if empirical potentials are transferable.

In comparison with the parallel interpretation of motion which can be obtained by fitting the individual ADPs, a way which is presently preferred by most crystallographers, the main difficulties of our theoretical calculations are the need of adequate knowledge of empirical potentials, which still have to be developed for many groups of substances, and the harmonic approximation, since no satisfactory model of this kind has yet been developed for anharmonic motion.

However, at least in some problematic instances (pyrope, almandine), where anharmonic behaviour has long been claimed, joint examination of crystallographic and thermodynamic properties compared with the theoretical model has provided a consistent explanation based on harmonic motion and order-disorder transformations.

MS11.06.04 ANALYSIS OF ANISOTROPIC DISPLACEMENT PARAMETERS IN A SERINE PROTEASE Th.R. Schneider, European Molecular Biology Laboratory (EMBL), c/o DESY, Notkestr. 85, 22607 Hamburg, F. Parak, Faculty of Physics, E17 of the Technical University Munich, 85748 Garching

Based on X-ray diffraction data to atomic resolution the structure of a serine protease has been determined at 90, 120, 180 and 300 K. Refinements were performed employing restrained anisotropic displacement parameters (ADP's) as implemented in the program SHELXL93¹. After convergence several cycles of block-matrix least-squares refinement were run to determine estimated standard deviations for coordinates and displacement parameters. Graphical inspection of vibrational ellipsoids revealed that significant anisotropy in atomic displacements can frequently be found for solvent exposed sidechains and carbonyl oxygens. Numerical analysis of the ADP's originated from the evaluation of the rigid-body test² whereby extended parts of the polypeptide backbone were detected as 'potentially rigid'. Fits of physically constrained TLS-models to these regions allow the explanation of parts of the individual atomic displacements in the protein molecule by a temperature dependent disorder of the molecule as a whole. It must be emphasized that, since internal normal modes are not considered in a pure TLS-analysis, the derived magnitudes for the TLS-terms only represent upper limits to the real values^[3]. The remaining contributions to the ADP's can be linked to conformational substates, internal dynamics and zero-point motions.

¹G.M. Sheldrick; SHELXL-93; University of Goettingen (1993)

²R.E. Rosenfeld et al.; Acta Cryst. A34:828-829 (1978)

³A. Kidera and N. Go; J.Mol.Biol. 225:457-475 (1992)

MS11.06.05 ANISOTROPIC VIBRATIONAL ANALYSIS OF THE SMALL PROTEIN CRAMBIN. Martha M. Teeter* and Boguslaw Stec. Department of Chemistry, Boston College, Chestnut Hill, MA 02167. *Sabbatical address: Max Planck Institute for Biophysics, 60528 Frankfurt/Main, Germany.

Full Matrix Least Squares refinement of the small protein crambin (4.7 kDa, 46 residues) at 0.83 resolution and 130K permits full anisotropic refinement of most atoms in the protein (Stec, Zhou and Teeter, (1995) Acta Cryst. D51, 663-681). With the program RFINE, the protein can be refined by the small molecule

vibrational method of TLS refinement (Schomaker, V. and Trueblood, K. (1968) Acta Cryst. B24, 63-76). This refinement can show how well the atomic displacement for the protein atoms are modeled by rigid body movement. It can also indicate non-rigid body motion, such as disorder, and aid in determination of external or lattice contributions to the anisotropic vibration factors.

Better agreement with individual B value refinement is found with three-rigid bodies rather than with two or one. However, the deviations in single rigid body B values from the individual B values are found to occur at disordered residues. This means that such a plot can be useful to indicate disorder, modeled or unmodeled.

We have used TLS to estimate the percentage of the B values that is due to external vibration. In this approach, we modeled the protein as one rigid body, two rigid bodies and three rigid body. We hypothesized that the common parts of the tensors for these three descriptions would represent the external or lattice contribution to the vibrational factors. This leads to the conclusion that 60% of the motion is external. This is in agreement with Diamond's refinement of a protein using by normal modes (Diamond, R. (1990) Acta Cryst. A46, 425-435), where external vibration was found to dominate the B value.

MS11.06.06 RECOMMENDATIONS ON ADP NOMENCLATURE AND USAGE. Kenneth N. Trueblood, Department of Chemistry and Biochemistry, University of California, Los Angeles, CA 90095-1569, USA

Modern x-ray and neutron diffraction techniques can give precise parameters that describe dynamic or static displacements of atoms in crystals. However, confusing and inconsistent terms and symbols for these quantities occur in the crystallographic literature. The recommendations of a subcommittee appointed by the IUCr Commission on Crystallographic Nomenclature concerning these quantities will be described. The report of this subcommittee is now under consideration by the IUCr Executive Committee. We anticipate that the entire report will be published in 1996, in *Acta Cryst.* A52.

The chief focus is on anisotropic atomic displacement parameters (ADPs) in the Gaussian approximation. The principal recommendations will be presented, with examples to illustrate their implications. These include:

— With the common Gaussian approximation, use either the quantities U_{ij} which have dimension (length)², or the dimensionless β_{ij} (each of which will be defined). Avoid using those now usually symbolized as B_{ij} which are directly proportional to the U_{ij} , the ratio being $8\pi^2$.

— Avoid using the term "temperature factor", because the phenomenon represented may not be due entirely to thermal motion and because that phrase has been used in several distinct senses.

— Published values of U_{eq} should always be accompanied by their standard uncertainties. The ratio of the minimum to maximum eigenvalues of the corresponding anisotropic displacement tensors should also be published, either in the primary publication itself, or in the secondary (deposition) publication.

Authors of crystallographic software are encouraged to introduce the minor modifications needed to implement the subcommittee's recommendations.