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HYDROGEN BONDING IN RNA SYSTEMS VIEWED BY MOLECULAR DYNAMICS SIMULATIONS

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Molecular dynamics (MD) simulations have been found useful to describe many features of hydrogen bonds in nucleic acid and especially RNA systems. Some of them will be discussed like the stability of CH-O and bifurcated hydrogen bonds. An emphasis will be placed on the stability of the solute-solvent hydrogen bonds. MD simulations at three different temperatures (5, 25, and 37°C) have shown that the lifetime of such hydrogen bonds displays a significant temperature dependence. These temperature dependent simulations may shed some light on melting (high temperatures) and crystallization (low temperature) processes. Results from simulations of crystal lattice of RNA systems will also be presented (see **http:///www-ibmc.u-strasbg.fr/upr9002/westhof/**).

Keywords: MOLECULAR DYNAMICS SIMULATION NUCLEIC ACIDS TEMPERATURE DEPENDENCE

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GENERATION AND APPLICATION OF STRUCTURE ENVELOPES

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Using just a few strong reflections from the low-angle region of a powder diffraction pattern, a structure envelope can be generated. This special type of periodic nodal surface separates regions of high electron density from those of low electron density, and can be used to advantage in combination with direct-space approaches to structure solution. The structure envelope not only reduces the volume of the asymmetric unit in which a direct-space search should be conducted by a factor of approximately two, but its shape also imposes a severe geometric restriction. To generate an informative structure envelope, the phases of the structure factors of the reflections used must be determined, and an algorithm has been developed for this purpose. The program SayPerm combines (1) the use of error correcting codes (ecc's) to sample phase space efficiently, (2) a pseudo-atom approximation of structure fragments to simulate atomic resolution at ca 2.5 Å, and (3) phase extension and phase set ranking using the Sayre equation.

The beneficial effect of using a structure envelope in structure solution was first demonstrated in combination with the program FOCUS, a zeolite-specific structure determination program. Then extension to molecular structures in combination with a simulated annealing program was also explored. This resulted in the development of the program SAFE and the subsequent determination of the structure of a tri- β -peptide ($C_{32}N_3O_6H_{53}$) with 17 variable torsion angles.

Keywords: POWDER DIFFRACTION STRUCTURE ENVELOPES SIMULATED ANNEALING

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INDEXING AND STRUCTURE REFINEMENT - NEW FRONTIERS FOR CRYSTAL STRUCTURE DETERMINATION FROM POWDER DIFFRACTION DATA

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With the development of increasingly powerful direct-space algorithms for structure solution, powder indexing and structure refinement have emerged as new important bottlenecks for crystal structure determination from powder diffraction data.

A novel indexing algorithm, called X-Cell, will be presented that overcomes most of the problems currently encountered in powder indexing. X-Cell performs an exhaustive search within the defined parameter range and establishes a complete list of all possible indexing solutions. The zero-point shift of the powder diffraction pattern is determined as part of the indexing procedure. X-Cell is robust with respect to impurity peaks and the dominant component of phase mixtures may be indexed if high quality synchrotron data is at hand. The algorithm performs well for long and flat unit cells and is appropriate for all crystal systems.

The final structure refinement can be facilitated by the use of density functional theory (DFT) calculations. At fixed cell parameters, accurate atomic coordinates can be obtained by lattice energy minimization. The validity of the optimized crystal structure can then be verified by Rietveld refinement with fixed atomic coordinates. DFT calculations can also help to choose the correct crystal structure from a choice of possible structure solutions.

Keywords: POWDER INDEXING STRUCTURE SOLUTION DENSITY FUNCTIONAL THEORY

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INDEXING OF POWDER DIFFRACTION PATTERNS BY ITERATIVE USE OF SINGULAR VALUE DECOMPOSITION

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A fast and simple method for indexing powder diffraction patterns has been developed for large and small lattices of all symmetries. The method is relatively insensitive to missing high d-spacing reflections where on simulated data little effect in terms of successful indexing has been observed when one third of the d-spacings are removed. Comparison with two of the most popular indexing programs ITO12 and DICVOL91 have shown that the present method as implemented in the program TOPAS can successfully index simulated data where others fail. Also significant is that the present method performs well on typically noisy d-spacings comprising large diffractometer 2θ zero errors. Critical to its success the present method uses Singular Value Decomposition in an iterative manner for solving linear equations relating hkl's to d-spacings.

Keywords: INDEXING SINGULAR VALUE DECOMPOSITION POWDER DIFFRACTION