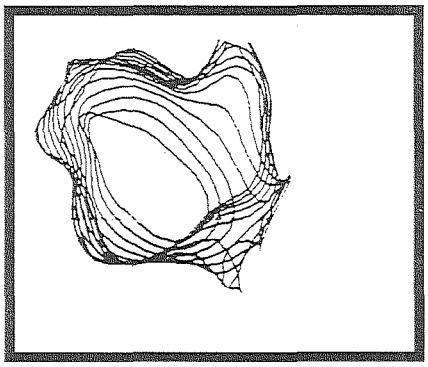
& Weber, *Nature*, 1988, 366, 403-405). The subunit of PCD from *P. aeruginosa* contains 438 residues, and that of *P. cepacia* 431. Both contain one nonheme iron atom. The identity between the two proteins is 48 percent, and there are many deletions and insertions. A conservative search model was used, consisting of 382 residues (1868 atoms) of a polyalanine (glycine) chain, from *P. aeruginosa*, with many gaps, and representing 1.6 percent of the unit cell contents of the *P. cepacia* PCD.

P. cepacia PCD crystallizes in $P2_12_12_1$ with four tetramers per cell. Ludwig *et al.* observed absences of odd orders of ℓ in the $hO\ell$ diffraction pattern, indicating the presence of a non-crystallographic local 2-fold axis at $x \approx 0.25$, and approximately parallel to *c* and suggesting that the local tetramer symmetry is 222. With a tetramer as the asymmetric unit, the rotational search with one monomer would normally give four symmetrically independent solutions. If a noncrystallographic 2-fold axis of the tetramer is parallel to a 2-fold axis in the Patterson, the rotation search solutions reduce to two correspondingly enhanced maxima. Thus the rotation search is facilitated by the orientation of the tetramer 2-fold axis. There is no corresponding enhancement of the maxima in the translation search.

With data to 2.9 Å resolution, the two maxima in the rotation search, mapped as the correlation coefficient, were 0.0809 and 0.0744, or 9.9 and 9.1 σ, respectively, in terms of standard deviations above the background. Spurious peaks were found at up to 3σ; among these were peaks resulting from an approximate 2-fold symmetry within part of the subunit (Ohlendorf *et al.*). The four symmetrically independent solutions to the translation search were found at 3.2 to 4.1σ; the known location of the non-crystallographic 2-fold axis made a fully exhaustive translation search unnecessary.

PS02.06.18 VERY LOW RESOLUTION PHASING ATTEMPTS OF THE RIBOSOMAL 50S PARTICLE FROM T. THERMOPHILUS BY THE FEW ATOMS MODEL METHOD. A.D. Podjarny, A.G. Urzhumtsev and E.A. Vernoslova, UPR de Biologie Structurale, IGBMC, B.P. 163, 67404 Illkirch Cedex, C.U de Strasbourg, France

A suggestion for the phases for the 80 Å resolution X-ray diffraction data from the 50S ribosomal particle of Thermus thermophilus (Volkmann et al., J. Mol. Biol., 216, 239, 1990) has been made using the Few Atoms Model ab initio technique (Lunin et al., Acta Cryst., D51, 896, 1995), in collaboration with A. Yonath and coworkers. This technique generated randomly one million models consisting of 5 pseudo atoms each and selected the 560 solutions which fitted best the observed amplitudes to 60 Å resolution. The selected models were grouped with a clusterisation procedure in a small number of possible solutions. The most adequate one was chosen by imposing the additional constraint that there should be no strong densities on symmetry axes. To refine this result, a second model generation was done imposing stronger amplitude constraints between 120 and 60 Å and density constraints based on the result of the first generation. The map resulting from the second model generation (phased to 80 Å) is shown in the figure. The position and features of the observed envelope agree with those obtained with other ab-initio solution methods and with molecular replacement using models from electron microscopy reconstructions (Volkmann et al., CCP4 Newsletter, 31, 23, 1995).



PS02.06.19 MOLECULAR REPLACEMENT METHOD USING A PARALLEL PROCESSING MACHINE. V.S.Yadava and K.K.Kannan Solid State Physics Division,Bhabha Atomic Research Centre,Bombay-400 085,INDIA.

The molecular replacement method involves six parameters - three rotational and three translational and the correct orientation and position is identified by calculating R-factor at each grid point.

Time requirement: The six-dimensional search requires very large amount of computer time. For a moderate size protien like Carbonic Anhydrase with about 2000 atoms in the molecule and 2000 reflections to 5A requires 20 minutes of cpu time on a Landmark 860 machine for structure amplitude calculations at 1.5Å resolution along the axes for each orientation. For a coarse search with steps of 5 degree in Eulerian angles there are 46656 orientations which require 648 days of computer time. However, with a 64-node parallel-processing system the time required is10 days of the machine time and can be further reduced by using more nodes and faster machines. Program implementation: As the calculations for each orientation are independent of that for others, the different orientations are equally distributed between different nodes. Each node has all the information for calculating structure amplitudes and Rvalue.

Results: The method has been tested first with Human Carbonic Anhydrase (HCA) I data and the same protein as model structure. Next HCA II was used as the model structure for obtaining structure of HCA I. Lowest R-value corresponded to correct orientation and position in both the cases.

PS02.06.20 AUTOINDEXING OF MULTIPHASE POLYCRYSTALS. V.B.Zlokazov FLNP JINR, 141980 Dubna, Moscow region, Russia. E-mail: Zlokazov@main1.jinr.dubna.su

Let a set of interplanar spacings (d_j), $j = 1,2,..,m$ be given, which are diffraction reflections from a *n*-phase polycrystal. The autoindexing problem is solved by minimizing the following functional

$$\sum_{i=1}^{n} \rho\left(\vec{d}, \vec{f}\left(\vec{P}_i, \vec{h}_i\right)\right) + \alpha V\left(\vec{P}_i\right) + \beta N\left(\vec{P}_i, \vec{h}_i, \delta\right) \quad (1)$$

The first member is

$$\rho = \sum_{j=1}^{m} \delta_1\left[d_j, f\left(\vec{P}_i, \vec{h}_j *\right)\right] \quad (2)$$

where $\vec{h}_j *$ = index values, minimizing expressions

$$R_j = \delta_2\left[d_j, f\left(\vec{P}_i, \vec{h}_j\right)\right] \quad (3)$$

and $f(\bar{P}_i, \bar{h}_j)$ is a formula, describing reflections; d_1 and d_2 are uadratic, or robust, or entropy metrics. At the same time $\bar{h}_j$ * , computed while minimizing R_j, index jth reflections. V and N are volumes of a phase and total number of reflections at tried parameter vectors.

The minimization of (1) with respect to $\bar{P}_i$ is carried out by trying parameter values from a assumed region, and refining them by analytical fitting, which, in case of convergence, gives the best estimate, or, if initial guesses are good enough, by analytical fitting.

Reference: Zlokazov V.B. Comp.Phys.Comm.,1995,v.85,p.415-422.

PS02.06.21 PHASING THE CHOLERA TOXIN ELECTRON DIFFRACTION DATA USING THE MAXIMUM ENTROPY-LIKELIHOOD METHOD WITH NON-CRYSTALLOGRAPHIC SYMMETRY IMPOSED IN THE MICE COMPUTER PROGRAM. W.N. Nicholson and C.J. Gilmore, Department of Chemistry, University of Glasgow, Glasgow G12 8QQ, Scotland U.K.

We have already reported our experience with applying the maximum entropy-likelihood method to phasing the two-dimensional projection data for cholera toxin (Gilmore & Nicholson (1995). Transactions American Crystallographic Association, 31 In press.). We have been working with a 2-d data set for which 56 unique image phases are available at 8.8Å resolution, and for which a further 1417 diffraction intensities extend to 4Å. The problem has been:

1. To phase the 4Å data from the 56 known phases.
2. To impose 5-fold non-crystallographic symmetry on the projection.
3. To impose envelope and solvent flattening constraints.

The maximum entropy-likelihood program (MICE) has been modified to carry out these steps. Using it we have shown that the likelihood criterion to is an accurate and reliable predictor of:

4. The effective number of atoms in the unit cell.
5. The centroid coordinates for the 5-fold non-crystallographic axes.
3. The envelope radius.

We are now extending the procedure to phase data derived from a series of electron diffraction patterns derived from a limited set of specimen tilts. The extension of two-dimension phase information into three is non-trivial especially when so little a priori phase information is available, and will be discussed in detail.

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Metalloproteins X-Ray & EXAFS Studies

MS02.07.01 EXAFS STUDIES OF NITROGENASE AND RELATED SYSTEMS: AN OVERVIEW. Keith O. Hodgson, Department of Chemistry Stanford University, Stanford, CA 94305

X-ray absorption edge and extended fine structure (EXAFS) studies contributed significantly to the early definition of particularly the Mo- Fe-S containing cofactor (FeMoco) of the MoFe protein of the nitrogenase system both within and outside the protein (in its isolated form). The x- ray crystal stucture results have now defined the overall protein structure and the relationships and structures of the metal-containing prosthetic groups in the resting state. However, much remains to be learned about how the electronic structure of the FeMoco mediates electron transfer and dinitrogen reduction and XAS spectroscopy is now being used to probe this question. Edge studies provide information on electronic structure including covaleny and electronic distribution as a function of oxidation state. EXAFS results incorporating multiple scattering analyses provide a specific probe of the metrical details (including longer range distances) and in some cases geometry of the FeMoco. This talk will review some of these recent advances as they provide insights into the structure/function of the nitrogenase system.

MS02.07.02 EXAFS AND X-RAY STUDIES OF B_{12} MODEL COMPOUNDS. Christoph Kratky, Institut für physikalische Chemie, A-8010 Graz - Austria.

The chemical and structural complexity of the B_{12} coenzymes (5'-desoxyadenosyl cobalamin and methyl cobalamin) and their biologically relevant reactivities (Co-C bond homolysis and Co-C bond heterolysis, respectively) has been a puzzle ever since the elucidation of their structures by Dorothy Hodgkin's group more than three decades ago. For many years, the focus of structural and chemical research lay on the isolated cofactor or cofactor analogue, with special emphasis on the cobalt center and its coordination environment.

Along these lines, we have determined crystal structures of a number of cobalamins with different α- and β-substituents. Using synchrotron radiation in combination with imaging plate detectors for some of these analyses, we were able to collect very accurate and comprehensive data sets, which permitted structure refinement to a level of precision comparable to a well-determined small-molecule crystal structure. From the combined structural data of about 20 cobalamin crystal structures, correlations between several characteristic intra-molecular deformation parameters (upward-folding of the corrin ring, axial Co-N distance, orientation of the dimethylbenzimidazole base) can be established and used to estimate the relative "stiffness" of each of these deformation modes.

In recent years, the B_{12} field has advanced dramatically as a result of the elucidation of the first crystal structures of proteins binding a B_{12} cofactor (B_{12} binding domain of methionine synthase; methylmalonyl CoA mutase). In both proteins, a protein-derived histidine-imidazole occupies the α-axial coodination of the cobalt center, replacing the dimethylbenzimidazole base occupying this position in solutions of the isolated cofactor under physiological conditions. Thus, it appears that some of the above structural correlations refer to a biologically irrelevant cofactor constitution.

For a number of representative compounds, we have also collected X-ray absorption spectra as a basis for the interpretation of EXAFS spectra of cobalamins in „non-crystalline" environments (e.g. cobalamins in solution and bound to a protein). Thus, by a comparison of the spectra of Aquocobalamin perchlorate in solution and in crystalline form, we could show that there is no detect-