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### Title

RECONSTRUCTION OF GLUTAMINE-SYNTHETASE FROM ELECTRON-MICROGRAPHS BY COMPUTER AVERAGING

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**TU-AM-E3 QUADRUPOLE SPLITTING, OXYGEN GEOMETRY AND ELECTRONIC CONFIGURATION IN MODEL OXYHEME.** G. H. Loew, and R. F. Kirchner\*. Stanford Univ., Stanford, CA 94305

The electronic structure of model oxyferroporphyrin complexes with N-methylimidazole as an axial ligand have been calculated for twenty-two conformations of the di-oxygen ligands using the iterative extended Hucker method. A bent, end-on dioxygen ligand geometry with low energy off-axis displacements and a low energy barrier to rotation about the Fe-O axis possibly coupled to a large amplitude bending mode of the Fe-O-O bond is favored. The electric field gradient at the iron nucleus observed as quadrupole splitting in Mössbauer resonance was calculated for each dioxygen ligand geometry in six likely electronic ground-state configurations. A paired iron(II)-dioxygen configuration yields the large negative electric field gradient observed for oxyhemoglobin and synthesized model compounds. The observed temperature dependence may be accounted for by rotation about the Fe-O axis which are more hindered in the protein than in the model compound.

**TU-AM-E4 THE STRUCTURE OF X-RAY ABSORPTION EDGES: APPLICATION TO BIOINORGANIC COMPOUNDS.** S. Doniach, T. Eccles\*, K. Hodgson, F. Kutzler\*, D. Misemer\* & R. Natoli\*. Stanford University, California 94305.

Semiempirical numerical fits of data taken at Stanford Synchrotron Radiation Laboratory on a variety of Cu model compounds and on hemocyanin(Hc) allow a classification of features at the K-shell xray absorption edge in terms of bound excitation-like levels, continuum threshold, and resonance peaks in the continuum. The positions and strengths of these features correlate closely with the chemical oxidation state of the Cu ion for model compounds and allow an unambiguous assignment of Cu(I) and Cu(II) to both Cu ions in deoxy Hc and Oxy Hc respectively. The observed binding energies will be correlated with results of calculations using a multiple scattering treatment of the Schrödinger equation for small atomic clusters. Preliminary results show a dependence of binding energy on site symmetry for a cluster of given composition and oxidation state.

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+Research partly supported by NSF Grant PCM 78-17105.

**TU-AM-E5 STEREOCHEMISTRY OF ANTITUMOR DRUG-NUCLEIC ACID BINDING: STRUCTURE OF ELLIPTICINE-5-IODOCYTIDYL(3'-5') GUANOSINE CRYSTALLINE COMPLEX.** S. C. Jain, K. K. Bhandary and H. M. Sobell, Departments of Chemistry and Radiation Biology & Biophysics, University of Rochester, Rochester, N.Y. 14627.

Ellipticine, a plant alkaloid possessing high activity against mouse leukemia L1210, forms a crystalline complex with self complementary dinucleoside monophosphate, 5-iodocytidyl(3'-5')guanosine(iodoCpG). The crystals are monoclinic, space group P2<sub>1</sub> with cell dimensions a=13.88, b=19.11, c=21.42 Å and β=105.43°.

We have solved the three dimensional structure of this complex by Patterson and Fourier techniques and presently it is being refined by Fourier and Least squares methods. The asymmetric unit in the structure consists of two iodoCpG, two ellipticine, 15 water and two methanol molecules, a total of 139 non-hydrogen atoms. The R factor at the present stage of refinement is 0.22. The structure demonstrates ellipticine intercalation into a miniature Watson-Crick type double helix formed by two iodoCpG molecules. As in ethidium-dinucleoside crystalline complexes, a mixed sugar puckering pattern of the type C3'endo(3'-5') C2'endo has been observed. Other details will be presented.

**TU-AM-E6 RECONSTRUCTION OF GLUTAMINE SYNTHETASE FROM ELECTRON MICROGRAPHS BY COMPUTER AVERAGING.** J. Frank\*, W. Goldfarb, M. Kessel\*, D. Eisenberg and T. S. Baker, Div. of Labs. & Res., NYS Dept. of Health, Albany, NY 12201 and Molecular Biology Institute, UCLA, Los Angeles, CA 90024

The structure of glutamine synthetase molecules from the bacteria *B. caldolyticus* and *E. coli* has been studied by using electron microscopy combined with computer averaging for low( $1e/\text{Å}^2$ ) and high ( $200 e/\text{Å}^2$ ) electron dose and various conditions of stain. The particles which are dodecamers are found to adhere predominantly to the carbon support film by their flat faces, appearing as rosettes with six-fold symmetry. Groups of 64 individual particles are selected from micrographs and scanned into 70 by 70 arrays using the Perkin Elmer flatbed microdensitometer. For each group, an average particle is computed after orientations and translations are determined using correlation functions <sup>1</sup>/1,2/.

/1/ Langer, R., Frank, J., Feltynowski, A., and Hoppe, W. Ber. Bunsenges. Phys. Chem. **74**, 1120 (1970).  
/2/ Saxton, W. O. and Frank, J., Ultramicroscopy **2**, 219 (1977).

**TU-AM-E7 DYNAMIC LASER SCATTERING STUDIES OF HUMAN AND BOVINE CERVICAL MUCUS.** W.I. Lee, P. Verdugo and R.J. Blandau\*. Dept. of Biological Structure and Center for Bioengineering, SM-20, University of Washington, Seattle WA, 98195.

We have proposed that the molecular arrangement of cow estrous cervical mucus and human midcycle cervical mucus is composed of an ensemble of entangled random-coiled macromolecules instead of a fibrillar crosslinked network (Bull. Amer. Phys. Soc., **22**:397, 1977). This report describes the studies of these macromolecules by laser light-scattering. Upon dissolving in a large amount of physiological saline by gentle and slow agitation with stirrer, macromolecules of bovine cervical mucus have a value of diffusion coefficient higher than that of macromolecules of human cervical mucus ( $D_{\text{bovine}} = 0.56 \times 10^{-8} \text{ cm}^2/\text{s}$ ;  $D_{\text{human}} = 0.38 \times 10^{-8} \text{ cm}^2/\text{s}$ ). *In vitro* observations of the migration of human spermatozoa in bovine and human cervical mucus suggest that the size of cervical macromolecules has definite effect on the flagellation and penetrability of spermatozoa.

This work is supported by NIH Grant HD-03752 and Contract HD-42826.

**TU-AM-E8 THERMODYNAMICS OF GLYCOSYL ISOMERIZATION IN CYCLIC AMP.** F. Jordan, P. R. Hemmes\*, and L. Oppenheimer\*, Chemistry Department, Rutgers University, Newark, New Jersey 07102

Ultrasonic relaxation measurements were performed on adenosine-3',5'-cyclicmonophosphate in water and in 7 M urea. The relaxation was attributed to the glycosyl C-N conformational equilibrium. The apparent thermodynamics and kinetic properties, calculated from the relaxation data, were different in 7 M urea than in water. A detailed analysis of the results showed that the glycosyl conformational and stacking equilibria are strongly coupled but in 7 M urea the effects of base stacking no longer intervene. The magnitude and sign of the thermodynamic quantities calculated in 7 M urea can be rationalized by a solvation model in which the ribosephosphate moiety is less solvated in the syn than in the anti conformation. The conformational equilibrium constant is ca. 4 near ambient temperatures.