075. HYDRODYNAMIC STUDY OF CARBOXYMETHYL CHITIN. E.V.Korneeva, G.A.Vichoreva, S.E.Harding and G.M.Pavlov, Institute of Macromolecular Compounds, St.Petersburg, 199004, Russia; NCMH, University of Nottingham, LE12 5RD, UK.

Carboxymethyl chitin samples (CMCh) were prepared by alkylation of chitin from crab and krill with monochloroacetic acid in isopropanol in the presence of NaOH. The preparations of CMCh were investigated by hydrodynamic methods in NaCl containing phosphate-chloride buffer solution (pH=7.0, I=0.20M) at 25°C. In this solvent the ionic strength is sufficiently high so that primary polyelectrolyte effects are not significant. Intrinsic viscosities, translational diffusion and sedimentation coefficients and the sedimentation concentration dependence coefficients were all measured. Molar masses ($44<(M_{SD}\times10^{-3})<239$) of samples were also estimated on the basis of sedimentation-diffusion analysis: the combination of M with the various translational characteristics referred to above allows us to establish the corresponding scaling correlations for CMCh. The equilibrium chain rigidity can be also estimated. Sizes of CMCh chains were compared to those of previously studied soluble chitin derivatives and other water-soluble polysaccharides. The support of Russian FFR (96-03-33847a).

076. AN OVERVIEW OF CHEMOMETRIC TOOLS FOR MULTIVARIATE CHARACTERIZATION AND CALIBRATION

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In the course of the past two decades, chemometrics has developed into a scientific field of its own. This is mostly due to the emergence of multivariate analysis methods using projection as a means to summarize complex, multi-dimensional information, thus reducing it to a small number of so-called latent variables. This talk outlines the basic principles underlying all projection methods, and focuses on three classes of applications. As a first step in data modeling or as a stand-alone method, PCA is a powerful exploratory tool. Regarding regression, the PCR and PLS methods are introduced, and compared to the more classical M.L.R. Lastly, SIMCA classification and PLS Discriminant Analysis address characterization or identification problems.

077. TARGET TRANSFORMATION FACTOR ANALYSIS AS A TOOL FOR THE INTERPRETATION OF LOADING SPECTRA

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For several years principal component analysis (PCA) has been used for finding the number and the nature of principal components in the data. The disadvantage of standard PCA is, that the resulting components are pure mathematical abstract factors with usually little or no physical or chemical meaning. Target transformation factor analysis (TTFA) allows to find physically significant factor loadings to facilitate the interpretation of complex spectra. The idea is to use the known chemical background information for finding chemically meaningful factors by rotating the orthogonal principal components to known spectra which are supposed to be part of the system. In addition, this procedure allows to project the rotated loading spectra to a given response similar to PLS but the resulting factors are real spectra which describe the response. This is then called target projection regression (TPR). Some examples are given on the use of TTFA respectively TPR to interpret NIR- and MIR- spectra of lignins and cellulosic materials. The results are compared to standard PCA/PLS as well as to a classification with a neural net.