22.4-1 SMALL ANGLE X-RAY SCATTERING FROM COAL. By M.H. Reich, I.K. Snook, and H.K. Wagenfeld, Department of Applied Physics, Royal Melbourne Institute of Technology, Melbourne, Victoria, Australia.

X-ray scattering from coal samples exhibits curvature when plotted on Guinier and Porod plots. This can be attributed to the polydispersity of the size and shape of the pores in the coal sample. Because of this, the determination of pore parameters cannot be undertaken using a Guinier or Porod analysis. The approach we have pursued is to model the size distribution of the pores using a Maxwellian distribution and best fit the data using three "extreme shapes" (spheres, ellipsoids of zero and infinite eccentricity). Along with knowledge of the absolute intensity of the scattering, these best-fit distributions can be used to determine the approximate volume and surface area of the pores and as well as indicate the sensitivity of these values to assumptions about the pore shape.

22.4-2 SMALL-ANGLE SCATTERING OF POLY(SODIUM ASPARTATE) SOLUTIONS. By J. Plestil, Yu. Ostanevich, D. Hlavat&yacute;, V. Saudek, Joint Institute for Nuclear Research, Dubna, USSR and Institute of Macromolecular Chemistry, Czechoslovak Academy of Sci., Prague 6, Czechoslovakia.

Aqueous solutions of poly(sodium aspartate) (c = 0.01-0.15 g/cm³) were studied by means of small-angle X-ray scattering. Scattering curves have a maximum, the position of which moves towards larger values of momentum transfer (h = (4π/λ)sinθ) with increasing concentration. For the polyelectrolyte studied, the dependence hmc1/3 has been observed, contrary to the behavior of other linear polyelectrolytes and to the predictions of cylindrical and isotropic models (P. de Gennes et al., J. Physique (1976) 37, 1451), according to which an exponent 1/2 is expected. Scattering data are interpreted in terms of a modified cylindrical model, using the scattering factor of individual molecules. Experimental inter-polyion distances (3-9 nm) are higher than the values obtained from volume balance assuming fully extended chains (2-7 nm). A possible explanation is that the length per one repeat unit of real polyanion is about one half the value corresponding to a fully extended polyanion.

The existence of the maximum on scattering curves of polyelectrolytes can be explained without introducing assumptions about the regular arrangement of polyanions (M. Bennouna et al., J. Physique (1982) 43, 1779; H. Koyama, Physica (1983) 120B, 418). An attempt will be made to interpret the scattering curves of poly(Na Asp) in terms of formulae given by Koyama.

22.4-3 SAXS STUDY OF STRUCTURE OF SOME SNAKE TOXINS. By J.R. Beltran, A.F. Craievich, Y.P. Mascarenhas, Instituto de Fisica e Quimica, C.P. 369, 13580, S. Carlos, S.P., Brazil and C.J. Laure, Faculdade de Medicina de Ribeirao Preto, 14100, Ribeirao Preto, S.P., Brazil.

Crotamine and crotoxin are neurotoxins isolated from the Brazilian snake Crotalus durissus terrificus. Crotamine is a polypeptide toxin, strongly basic (pH=10.3), with molecular weight of 3870 daltons. It is composed of 42 residues of 15 common amino acids including six half-cystines. It has a very high lysine (9 residues) and low arginine (2 residues) content. The N-terminus is tyrosine and the C-terminus glycine.

Crotoxin is a complex toxin formed by the association of two proteins: a phospholipase (molecular weight = 15,700 daltons) and crotapotin (molecular weight = 4,000-4,500 daltons). The radii of gyration of crotamine, crotoxin, phospholipase and crotapotin were determined by the small-angle X-ray scattering technique. Several molecular solutions have been studied to correct for concentration effects. The apparent molecular radius of gyration of crotamine is also determined as a function of pH and an important change at pH between 9.5 and 12.5 is attributed to a dominant effect of molecular aggregation. The radii of gyration of crotoxin, phospholipase and crotapotin are respectively equal to 18.4, 15.2, and 14.7 Å.

This work was sponsored by CNPq, FAPESP, and FINEP.

C - 478 22. GASES, LIQUIDS AND AMORPHOUS COMPOUNDS