13. NEUTRON DIFFRACTION


Small-angle neutron scattering (SANS) experiments were performed on poly(ethylene terephthalate) (PET) with the Oak Ridge National Laboratory 30-m SANS instrument. An improved sample preparation technique which produces void free films was developed. Single chain dimensions in amorphous undrawn films were measured for different label (deuterated chain) concentrations. The SANS radius of gyration was compared to the theoretical value and the molecular weight was compared to the GPC molecular weight. The extent of the order-disorder reaction, both in the solid and the melt (temperatures from 200 to 300°C), was measured by following changes in the scattering curves over a period of time. Preliminary experiments on drawn PET samples were also performed as background for future work.

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13.5-2 WATER MOLECULES IN NATURAL ZEOLITES STUDIED BY NEUTRON DIFFRACTION*. By A. Knick, Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973 and G. Artioli, J. J. Pluch and J. V. Smith, The Department of Geophysical Sciences, The University of Chicago, IL 60637.

A series of neutron diffraction experiments using natural zeolites have been performed at the Brookhaven National Laboratory High Flux Beam Reactor in order to study the bonding of the water molecules and the cations in the zeolitic cavities. The ultimate aim of the studies is to develop models that will be useful for the understanding of reversible dehydration and ion-exchange properties of zeolite molecular sieves.

Precise structural data for natrolite, edingtonite, thomsonite and brevosterite collected in the temperature range 20K to 623K have yielded important information on the water molecules and their interaction with the cations and the framework oxygens. The hydrogen bonding is usually weak and the molecules adapt well to the local charge distribution in the framework. The 0...0 distances vary in the ordered zeolites between 2.68 Å to 3.02 Å with 0...0...0 angles between 140 to 176°. The stronger bonds are accepted by oxygen atoms bonded to both Si and Al. In brevosterite there is Si/Al and cation disorder a complex hydrogen bond schema is observed. The water oxygen atoms have fixed positions whereas the hydrogen atoms assume alternative positions to adjust to the varying local charge distribution caused by the disorder.

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