

s9.m1.p3 **From Polyaniline Oligomers to Conducting Organic Crystals.** A. Gawlicka-Chruszcz¹, K. Stadnicka^{*)}, J. Laska^{**)}, *Faculty of Chemistry, Jagiellonian Univ., ul. Ingardena 3, 30-060 Kraków, Poland; Faculty of Materials Science and Ceramics, Univ. of Mining and Metallurgy, al. Mickiewicza 30, 30-059 Kraków, Poland.*
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Although polyaniline is known since 1862, its transport properties brought about a rediscovery of this organic polymer nearly 10 years ago. The basic form of polyaniline is not conducting, but its protonated forms display a tenfold increase of the specific conductivity. Macroscopic conductivity of a polymeric sample is a complicated function of many parameters, of which the most important are microscopic conductivity along the polymer chain and degree of crystallinity. It also depends on sample morphology.

Single crystals of polyaniline are difficult to obtain. Therefore, the crystalline structure of polyaniline in the form protonated with camphorsulfonic acid, i.e. emeraldine, was subjected to computer modelling and calculated powder diffraction pattern was compared with the experimental results¹. The model structures consist of layers of parallel polyaniline chains intercalated by camphorsulfonic acid molecules.

In the present work a different strategy was used. The project is devoted to the synthesis, crystal growth and structure analysis of various forms (with different degrees of protonation and increasing chain length) of polyaniline oligomers, to be correlated with physical properties of the obtained crystals. First N,N'-diphenyl-p-phenylenediamine was chosen as simple polyaniline oligomeric form and acids, such as p-toluenesulfonic and camphorsulfonic, were used as protonating agents. X-ray structure analysis of the obtained single crystals was performed. Main features of these simple structures are going to be used in designing polyaniline-based crystalline organic conductors.

s9.m1.p4 **Phases of Solid Methanol.** B.H. Torrie¹, O.S. Binbrek², I.P. Swainson³, ¹*University of Waterloo, Canada,* ²*King Fahd University of Petroleum and Minerals, Saudi Arabia,* ³*NRC, Canada.*
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Methanol is known to have an ordered orthorhombic structure, space group $P2_12_12_1$, below 157.4 K¹, and a disordered orthorhombic structure, space group $Cmcm$, between 157.4 K and the melting point at 175.37 K². There was evidence in the earlier work¹ that a metastable phase could be produced by rapid quenching of the high temperature phase.

Neutron powder diffraction patterns were recorded for both known phases and an effort was made to obtain the metastable phase. Quenched samples again gave observed powder diffraction peaks which could not be indexed with either of the known phases but these peaks were weak and few in number so the space group of the metastable phase could not be identified.

The structure of the high temperature phase was determined with x-rays in the 1950's² so only the positions of the carbon and oxygen atoms were found. The current results confirm the space group and give the positions of all of the atoms. A wide-angle detector allowed the diffraction pattern to be recorded quickly before preferred orientation developed.

The carbon and oxygen atoms are located on 'mm' sites and the molecules have a corresponding pseudo-symmetry which comes about as a result of a 180° flipping motion about the C-O axis. The time scale of the flipping motion is such that it gives rise to a large diffuse scattering background. Results of an analysis of the Bragg peaks and the diffuse background will be presented.

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