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EXAFS Studies of AsF_5 in Polyacetylene $(CH)_x$*. T. C. CLARKE, W. D. GILL, P. M. GRANT, H. MORAWITZ, G. B. STREET, IBM Research Laboratory, San Jose, CA 95193, and D. SAYERS, North Carolina State University, Raleigh, NC--We have performed extended x-ray absorption fine structure studies (EXAFS) between 300°K and 86°K on the As-K edge to understand the great change in the transport properties of polyacetylene $(CH)_x$ on intercalation with AsF_5. These experiments were performed utilizing synchrotron radiation at the Stanford Synchrotron Radiation Laboratory.* The gas phase AsF_5 edge and EXAFS spectrum were used as standards. We find substantial enhancement of the gas phase exciton features in the As edge structure in $(CH(AsF_5)_y)_x$. The As-F bond distances derived from the gas phase and polymer matrix are in agreement with existing measurements. The changes in the As-K edge structure will be discussed with regard to the amount of charge transfer from the $(CH)_x$ chains to the AsF_5 molecules and structural information derived from the As radial distribution function will be presented.

*With financial support of the NSF (under contract DMR-772-7489) in cooperation with the Department of Energy and the ONR.

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SESSION EI: POLYMERIC CONDUCTORS
Tuesday afternoon, 28 March 1978
Richmond Room, Sheraton-Park at 12 Noon
A.J. Heeger, presiding

EI 1 Exafs Studies of Brominated Polysulfurnitride* H. MORAWITZ, W. D. GILL, G. B. STREET, IBM Research Laboratory, San Jose, CA 95193, and D. SAYERS, North Carolina State University, Raleigh, NC--We report on extended x-ray absorption fine structure (EXAFS) studies of the bromine K-edge in brominated polysulfurnitride utilizing synchrotron radiation at the Stanford Synchrotron Radiation Laboratory*. The measurements were performed with the conducting b axis of the $(SNBr_{0.4})_x$ sample and the x-ray polarization vector parallel. Additional measurements were performed by rotating the sample to probe for contributions to the radial distribution function from SN units. We will also present the temperature dependence of the EXAFS and edge fine structure between 300°K and 86°K, which was studied to look for rearrangement of the incorporated bromine relative to the $(SN)_x$ lattice and anisotropic thermal motion of the bromine. The edge structure of the bromine K edge in $(SNBr_{0.4})_x$ will be discussed for its implications on the charge transfer and models presented for incorporated Br on the basis of the bromine radial distribution functions.

*With financial support of the NSF (under contract DMR-772-7489) in cooperation with the Department of Energy and the ONR.

EI 2 Temperature dependence of the paramagnetism in brominated $(SN)_x$. J.C. SCOTT,* J.D. KULICK,* Cornell University, Ithaca, NY and G.B. STREET, IBM Research, San Jose, CA. The static magnetic susceptibility of $(SN)_x$ doped with various amounts of bromine $[(SNBr_y)_x$ where $0 \leq y \leq 0.4]$ has been measured as a function of temperature. For y = 0, the susceptibility is temperature independent and the paramagnetic contribution (i.e. the measured value adjusted by Pascal's constants) is $\chi_p = (5.5 \pm 1.0) \times 10^{-6}$ emu/mole. For y = 0.40 the low temperature ($T \leq 30K$) data shows a small Curie-like contribution which can be used to put an upper limit on the concentration of $S = \frac{1}{2}$ species, such as $(Br_2)^-$, of 2×10^{-4} molar. At higher temperatures the brominated samples reveal a dependence on temperature which is closely linear: $\chi_p = \chi_o(y) + \alpha(y)T$, with χ_o and α both monotonically increasing functions of y. $\chi_o(0.40) = (16.9 \pm 1.2) \times 10^{-6}$ emu/mole and $\alpha(0.40) = (1.1 \pm 0.1) \times 10^{-8}$ emu/mole K. The detailed behaviour of the excess paramagnetism weighs against an interpretation in terms of band structure effects. Other possible mechanisms, such as Van Vleck paramagnetism and quantum degeneracy effects, will be discussed.
*Supported by NSF through Cornell MSC.

EI 3 Thermoelectric Power of Polysulfurnitride $[(SN)_x]$ at Very Low Temperatures. W. W. FULLER, P. M. CHAIKIN,† L. J. AZEVEDO,** W. G. CLARK, and J. HAMMANN, Physics Dept., U. of Cal., Los Angeles. -- Measurements of the thermoelectric Power (S) of $(SN)_x$ are reported for the temperature range $0.1<T<4.2K$ with a magnetic field of 0-15 kOe applied parallel and perpendicular to the $(SN)_x$ fibers. Above 1.2K a phonon drag term ($S \propto T^3$) is dominant. The superconducting transition ($T_c \sim 0.3K$) is observed in zero applied field. Below 1K the behavior in a magnetic field is complicated. It shows the effects of both superconductivity and magnetic impurities.

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EI 4 Very Low Temperature Thermal Conductivity of Polysulfur Nitride, $[(SN)_x]$.* L.J. AZEVEDO** and W.G. CLARK, U.C.L.A.--The thermal conductivity, κ, of polysulfur nitride, $[(SN)_x]$, has been measured from 0.08 K to 4 K in fields up to 18 kOe. The high temperature ($T > 0.5$ K) thermal conductivity is dominated by a field independent phonon contribution that varies from a T^3 temperature dependence at low temperature to an approximately linear temperature dependence at higher temperatures. For $T \sim 1.5$ K, where the specific heat is known, the phonon mean free path is on the order of the smallest sample dimension. Below 0.5 K, in addition to a dominant phonon part, a small contribution to κ due to electrons is observed. This contribution is identified by its magnetic field dependence. In the normal state, the electronic contribution to κ is the same as that calculated from the Wiedemann-Franz law using the measured resistivity.
* Supported by NSF Grant No. DMR-73-07612.
**Present Address: Sandia Laboratories, Albuquerque, New Mexico 87115.

EI 5 * EXAFS Studies of AsF_5 in Polyacetylene $(CH)_x$. T. C. CLARKE, W. D. GILL, P. M. GRANT, H. MORAWITZ, G. B. STREET, IBM Research Laboratory, San Jose, CA 95193, and D. SAYERS, North Carolina State University, Raleigh, NC--We have performed extended x-ray absorption fine structure studies (EXAFS) between 300°K and 86°K on the As-K edge to understand the great change in the transport properties of polyacetylene $(CH)_x$ on intercalation with AsF_5. These experiments were performed utilizing synchrotron radiation at the Stanford Synchrotron Radiation Laboratory.* The gas phase AsF_5 edge and EXAFS spectrum were used as standards. We find substantial enhancement of the gas phase exciton features in the As edge structure in $(CH(AsF_5)_y)_x$. The As-F bond distances derived from the gas phase and polymer matrix are in agreement with existing measurements. The changes in the As-K edge structure will be discussed with regard to the amount of charge transfer from the $(CH)_x$ chains to the AsF_5 molecules and structural information derived from the As radial distribution function will be presented.
*With financial support of the NSF (under contract DMR-772-7489) in cooperation with the Department of Energy and the ONR.

EI 6 Optical Properties of Doped Polyacetylene, W. BLUDAU, T. C. CLARKE, P. M. GRANT and G. B. STREET, IBM Research Laboratory, San Jose, CA--It has been recently reported that polyacetylene doped with AsF_5 exhibits conductivity levels generally associated with metallic or degenerate semiconductor behavior.[1] We have measured the reflectivity of cis-trans, trans- and AsF_5-doped trans-polyacetylene in the range 3000Å - 2.5μ as a function of temperature between 300K and 4.2K. Marked changes in optical properties occur upon doping polyacetylene with AsF_5, most notably the appearance of a reflectance edge beginning at 2.2 eV strongly suggestive of Drude-like excitations.
[1]C. K. Chiang, et al., Phys. Rev. Letters 39, 1098 (1977).

EI 7 Characterization of Doped Semiconducting Polyacetylene.* C.K. CHIANG, S.C. GAU, Y.W. PARK, A.J. HEEGER, and A.G. MAC DIARMID, Univ. of PA--We have studied the semiconducting polymer polyacetylene, $(CH)_x$, doped with various donors and acceptors. Acceptor doping includes halogens and AsF_5, and donor doping includes NH_3 and alkali metals. Using different dopants we are able to vary the electrical conductivity of doped polyacetylene from less than 10^{-10} $(\Omega\text{-cm})^{-1}$ to better than 600 $(\Omega^{-1}\,cm^{-1})$. Thermoelectric power measurements are used to obtain the sign of charge carriers and indicate n-type and p-type conduction for the donor and acceptor doped materials respectively. Initial doping to n-type (p-type) can be compensated by subsequent reaction with acceptors (donors).
*Supported by ONR.

EI 8 Infrared and Optical Properties of Doped Polyacetylene.* C.R. FINCHER, JR., Y. MATSUMURA, A.J. HEEGER, and A.G. MAC DIARMID, Univ. of PA--