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Relationship Between Structure and Properties for Donor-Doped and for Acceptor-Doped Polyacetylene

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RELATIONSHIP BETWEEN STRUCTURE AND PROPERTIES FOR
DONOR-DOPED AND FOR ACCEPTOR-DOPED POLYACETYLENE

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Abstract. Two basic structural types are experimentally derived for polyacetylene complexes: channel structures (Na, K, Rb, and Cs) and layered structures (iodine and a variety of other acceptors). Observed variants for the layered structures include first-stage and higher-stage complexes, with either complete or fractional occupation of dopant on the dopant-containing planes. A third structural type, in which dopant is statistically distributed, is predicted up to high dopant levels for lithium dopant. These structural results are used to explain observed properties and to predict properties obtainable for nearly defect-free single crystals. Discussions will include the structural origin of electrochemical discharge curves, major increases in conductivity on annealing K-doped and Rb-doped polyacetylene, the extremely high thermal stability of alkali metal channel complexes, and predicted mechanicals and transport properties for single-crystal complexes.