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"Design, Synthesis and Characteristics of Novel Polydiacetylenes Using New Analytical Techniques"

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Surface active diacetuler	ary and identify by block number) he where the electron	ic structure of the
sidegroups inductively couple	with the electronic	structure of the polymerized
backbone has been synthesized.	The fully polymeri	zed Langmuir-Blodgett
monolayers are expected to have	ve novel nonlinear op	tical properties. This
research is being pursued in 1	ight of significant	theoretical and experimental
findings established for singl	le crystalline polydi	acetylenes. In the
rolydiacetylenes that are bein	ng investigated, the	electronic structure of the
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Nonlinear optical properties of classes of polymers have recently received extensive attention. The possibility of their application in a number of optic techniques has led to new developments in material processing technologies and characterization and in anticipating new polymers with enhanced nonlinear optical properties. Large and fast third order nonlinearities have been reported for polymers such as Poly(benzbis-oxazoles), polyacetylene and polydiacetylenes¹. Polymers or composites with large second order effects have also been reported.

A large number of side groups may be synthesized and as a result of this variation in the side group structure one sees a tremendous variation in crystal morphology and extensive polymorphism for polydiacetylenes (PDA). This permits new approaches to their growth and processing. Two examples of these novel approaches are the use of Langmeir Blodgett film balance to grow diacetylene monolayers and thin film single crystal through solution techniques developed at GTE labs.

The diacetylene functionality is an extremely versatile vehicle for engineering at the molecular level. Polymerization in the solid state in a diacetylene monomer single crystal can be brought about by a variety of techniques including thermal and radiation induced polymerization. The polydiacetylene chain in the single crystal has a planar extended chain conformation and possesses a fully conjugated delocalized electronic structure. Extensive investigation has focussed on the 1-D electronic structure of these systems. Several ultrafast nonlinear optical signal processing schemes rely on a material's intensity dependent index of refraction as the basic nonlinear mechanism². In order to realize these concepts a material is needed with both a large and fast nonlinear optical coefficient with the additional requirement that the material is processible in the desired form (e.g. a waveguide). The PDA's possess one of the largest measured nonresonant third order nonlinear optical susceptibility and its response time has been measured to be no slower than a few femtoseconds.

On the basis of the properties of the PDA backbone alone one expects significant opportunities. The impact could be significantly broadened if in addition side group induced and initiated processes are included. Theoretical modelling by Tripathy and coworkers has indicated that attachment of side groups whose electronic structure can extensively renormalize the electronic structure of the backbone will substantially modulate the electronic properties of the backbone itself. From theoretical consideration dramatic possibilities are anticipated. Specific results from ongoing research and a broader overview of this emerging field of research will be presented.

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- 3.) Orchard, B.J and Tripathy, S.K. (1986) Macromolecules 19 1844.

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