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Opinion

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Polyacetylene in subnanometer channels

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Abstract:

A method is described for the preparation of polyacetylene in the channels of a urea inclusion compound. This involves the photochemical elimination of terminal iodine atoms from a conjugated diene, E, E-1, 4-diiodobuta-1, 3-diene (DIBD), which forms a commensurate and fully ordered compound with urea that has a stacked loop structure and block morphology. The DIBD guest is present in the urea host channel with the terminal iodine atoms of the guest molecules in Van der Waals contact. Photochemical cleavage of the terminal C-I bonds results in elimination of iodine from the single crystal material and the formation of a C-C bond to produce the conjugated tetraene and subsequent longer species. The loss of iodine is monitored by the weight loss. The new polyene species are monitored by Raman spectroscopy. With extensive irradiation the mass loss approaches that anticipated from the crystal stoichiometry and at the same irradiation time, the Raman intensity largely disappears. These features and the loss of intermediates show that the reaction proceeds to completion. The symmetry argument that predicts complete loss of Raman intensity for polyacetylene will be presented. Vibrational inelastic neutron scattering spectra in the urea-d4 host with varying degrees of irradiation will be presented and discussed. Replacement of the four carbon DIBD with the six carbon 1, 6-diiodohexa-1, 3, 5-triene (DIHT), made for the first time for this application, results in the formation of hexagonal needle crystals that are very similar to known dibromoalkane compounds. These DIHT-UIC materials make it possible to prepare composite materials in which the hexagonal channels will extend from one end of the crystal to the other using diffusional refilling of the channels as the polymer is elongated. It is anticipated that this composite material will be a one-dimensional superconductor that may find application as a magnetic energy storage device.

Biography:

Bruce S Hudson completed his BS and MS degrees in Chemistry at the California Institute of Technology and his PhD at Harvard University where he worked with Bryan Earl Kohler on the excited electronic states of linear conjugated polyenes. His thesis showed that the lowest excited electronic states of linear polyenes is not the HOMO to LUMO excitation but is instead a state of the same symmetry as the ground state and thus symmetry forbidden.

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