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Polymorphic hydrogen bonded, disordered and photoreactive crystals

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Studies in hydrogen-bonded molecular crystal polymorphism will be presented with emphasis on the effect of replacement of the exchangeable H by D on the relative stability of polymorphic forms due the zero point and thermal vibrational effects, the use of periodic density function computations of crystalline state vibrations to understand the observed isotope effects and the use of spectroscopic methods, Raman and vibrational inelastic neutron scattering, to test the computations. The case of barbituric acid will be emphasized. In this case, it has been found that the most stable crystal is the monoenol rather than triketo despite the fact that the enol in isolation is much higher in energy (Angew. Chem. Int. Ed. 2016, 55, 1309 –1312 and cited work.) Urea channel inclusion host guest crystals (UIC's) containing 1,4-diiodobutadiene as the guest is found (Cryst. Growth Des. 2013, 13, 3852−3855) to be commensurate and fully ordered, a rare but not unknown observation for this class of materials. The terminal iodine atoms are in contact in the channel. If these crystals are irradiated with UV light the iodine atoms are cleaved and oligo-diiodopolyenes are formed as indicated by Raman spectra. (Mater. Res. Soc. Symp. Proc. Vol. 1799 DOI: 10.1557/opl.2015.486). The crystal mass shows progressive loss of weight as the reaction proceeds. The product of this process will be polyacetylene. It has been anticipated that this material will be metallic without doping due to the lack of bond alternation. (J. Mol. Struct. 1032 (2013) 78–82). It may exhibit room temperature superconductivity.

Biography

Bruce S Hudson received his Bachelor's and Master's degrees from the California Institute of Technology in Chemistry and Biophysical Chemistry respectively and his PhD in Physical Chemistry from Harvard University in 1972. His thesis research with Roy Gordon involved the computation of inelastic neutron scattering spectra and that with Bryan E Kohler involved the electronic spectroscopy of linear conjugated polyenes. He is the author of over 200 publications and has served on NIH and NSF review panels.

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