Some diacetylene compounds are known to undergo solid-state polymerization upon heating, irradiation or mechanical stimulation, and give single crystals of conjugated polymer. The reactivity of a diacetylene in the crystalline state is governed by the packing of the monomer. Only those diacetylenes which have suitable packing conditions will undergo facile polymerization. The single crystals of these conjugated polymer have attracted attention on their physical properties, such as conductivity, optical nonlinearity, and mechanical strength.

We have investigated the correlation between the crystal structure and the reactivity in solid-state polymerization of various aromatic acetylene derivatives. We reported the crystal structures of some diethynylbenzene derivatives and interpreted the characteristic features of them in the solid-state polymerization upon irradiation with gamma-ray based on the unique monomer packings (Y.Kai, N.Yamamoto, D.Xu, K.Kashi, M.Higa, H.Yamamoto, T.Takahashi and K.Hayashi, Makromol. Chem. 1987, 188, 3047-3059). Recently, we have synthesized the aromatic diacetylene derivatives, 1-(5-hydroxypenta-1,3-diylnyl)-4-ethenylbenzene(I), 1,4-bis-(5-hydroxypenta-1,3-diylnyl)-benzene(II), and 1,2-bis-(5-hydroxypenta-1,3-diylnyl)-benzene(III), and obtained these single crystals. So the crystal structures of I, II and III were determined by X-ray diffraction method. As a result, it was found that the monomer molecules in the crystals of both I and II take suitable packing structures to undergo solid-state polymerization, but in the crystal of III, the monomer molecules are arranged not so as to undergo solid-state polymerization. With respect to the crystal of I, monomer arrangement is suitable for solid-state polymerization not only between diacetylene moieties but also ethynyl ones. The distance between the neighboring ethynyl moieties is nearer than that between diacetylene ones. So stepwise polymerization may be reasonable, first between ethynyl moieties, next between diacetylene ones.

The crystal structures of compounds of biopharmaceutical and technological uses, such as enzymatic inhibitors, antijuvemine hormones for plague control, bisaceties, useful polymers, compounds used in the leather industry, etc. A novel synthesis of 3-aroyloxypropiononitriles, avoiding the use of contaminants, has proved to give good yields for small substituents[1]. The compounds 2- and 4-(2-bromoethoxy)diphenylenethanes (I and II respectively) have been synthesized as part of a general study on the goodness of the synthetic method to handle bulkly substrats. No significant changes in the crystal structures of I and II have been observed in going from R.T. to 150K. The molecular conformation of I and II in solid state, obtained from single crystal X-ray diffractometric data at low temperature, are compared. The observed differences are analyzed and the conclusions correlated with solution R.T. H and 13C nmr data. Variations in the m.p. as a function of the substituents position are analyzed in terms of the different molecular packing.

PS06.00.18 STRUCTURAL STUDIES OF INTERMEDIATES IN A NOVEL SYNTHESIS OF ARYLOXY-PROPIONONITRILES. J. Ellenal3, G. Punet, J.C. Autino2, G.P. Romanelli2 and A.E. Goeta4. IPROFIMO. Dept. de Física, Facultad de Ciencias Exactas, UNLP, Argentina, 3IADECOM, Laboratorio de Estudio de Compuestos Orgánicos, Facultad de Cs. Exactas, UNLP, Argentina, 4Facultad de Ingeniería, UNLP, Argentina. 4Durham Chemical Crystallography Group, Chemistry Department, University of Durham, UK.

3-Aryloxypropiononitriles are important synthetic intermediates for compounds of biopharmacological and technological uses, such as enzymatic inhibitors, antijuvemine hormones for plague control, bisaceties, useful polymers, compounds used in the leather industry, etc. A novel synthesis of 3-aroyloxypropiononitriles, avoiding the use of contaminants, has proved to give good yields for small substituents[1]. The compounds 2- and 4-(2-bromoethoxy)diphenylenethanes (I and II respectively) have been synthesized as part of a general study on the goodness of the synthetic method to handle bulkly substrats. No significant changes in the crystal structures of I and II have been observed in going from R.T. to 150K. The molecular conformation of I and II in solid state, obtained from single crystal X-ray diffractometric data at low temperature, are compared. The observed differences are analyzed and the conclusions correlated with solution R.T. H and 13C nmr data. Variations in the m.p. as a function of the substituents position are analyzed in terms of the different molecular packing.