Abstract

Crystal and molecular structure of 2, 5 – bis(butoxy) 1,4-bis (biphengthethynyl) benzene and 2, 5-bis (Octyloxy) 1, 4-bis (biphenyl ethynyl) benzene :

S. A. Chawdhury[1], Paul R . Raithby [2] and Muhammad Younus [3]
Sylhet International University, Sylhet, Bangladesh.
University of Bath, U. K.
Shahjalal University of Science and Technology, Sylhet, Bangladesh.

Conjugated organic polymers are semiconductors which are used in wide range of devices such as light emitting diodes and photocells. Conjugated organic polymers have two major emissive states – singlets and triplets Radiative emission from triplet series is spin forbidden, so that only emission from the singlet state occurs. Recently the synthesis and investigation of spectrospic properties have been undertaken in Department of Chemistry, Shahjalal University of Science and Technology, Sylhet, Bangladesh and Department of Chemistry, University of Bath, U. K. The monomeric precursors have been structurally characterized by the single crystal X-ray crystallography. X-ray analysis of the two monomers (a) 2,5 – (butoxy) 1,4 – bis (biphenylethynyl)benzene, C_{42} H_{36} O_2 (b) 2,5 – bis(octyloxy) 1,4 – bis(biphenylethynyl) benzene, C_{50} H_{34} O_2 have been carried out to find the linear arrangements of the monomeric units in the polymers derived from them.

Crystal data of the compound (a) C_{42} H_{36} O_2, Triclinic, P1 with a = $\overline{9}$.2290 (3) A^0, b = 9.5120 (4) A^0, C = 19.2850(7) A^0 α = 99.206 (2) ^{0}. β = 100.980 (2)^0 γ = 105.393 (2)^0, Z=2, ρ_0 = 1.222 Mg/m^3, absorption coefficient 0.923 m m^{-1}, F (000) 612, crystal size 0.50 x 040 x 0.10 mm^3, teta range for data collection 2.98 to 27.60 ; final R = 0.0609 for 7130 independent reflections (b) C_{50} H_{36} O_2 is controsymmetric, monoclinic $P2_1/C$ with a = 16.8910(8) A^0, b, = 5.4580 (3) A^0, C = 22.6030 (13)A^0, β = 106.490, (2^0), Z=2, ρ=1.142 Mg/m^3, absorption coefficient o.667 nm^{-1}, F (000)=740, crystal size 0.45 x 0.15 x 0.03 mm, teta range for data collection 3.71 to 24.44 degrees. Final R indices 0.0577 for 3252 independent reflections.

Both structures were solved by direct methods and refined by full matrix least squares methods.

Keywords: X-ray, crystal structure, semiconductors