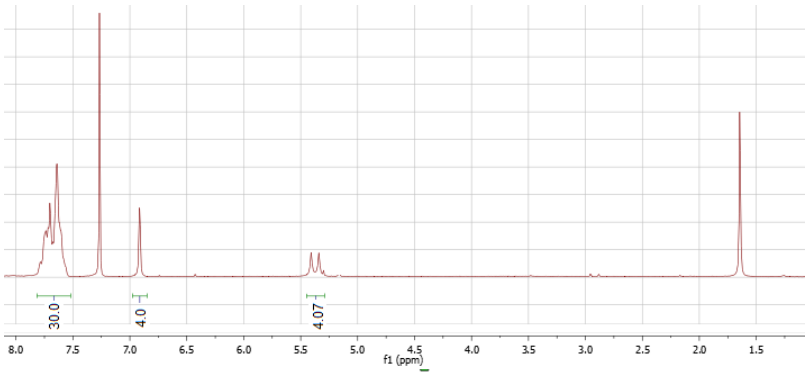
Electronic Supplementary Information

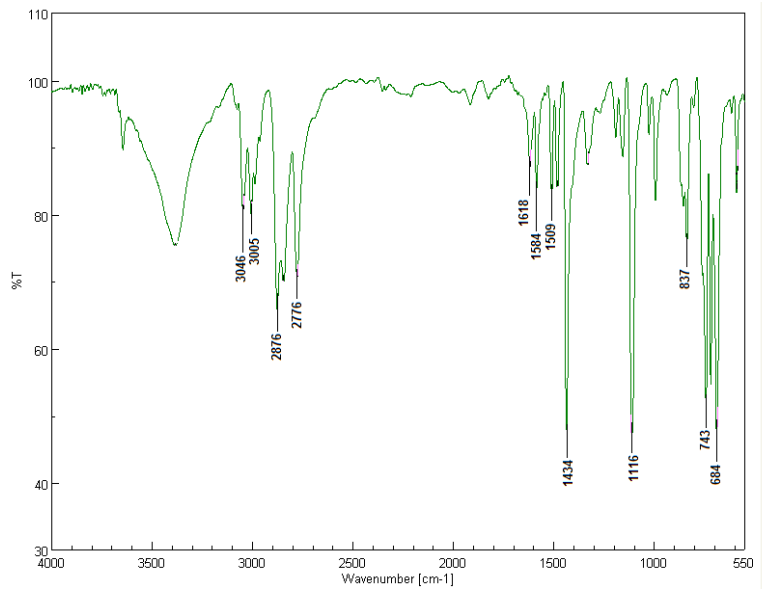
Title: Electronic and Structural Properties of Polymers Based in Phenylene vinylene and Thiophene Units. Control of Gap by the Gradual Increases of Thiophene Moieties.

Authors: C. O. Sánchez*, P. Sobarzo and N. Gatica

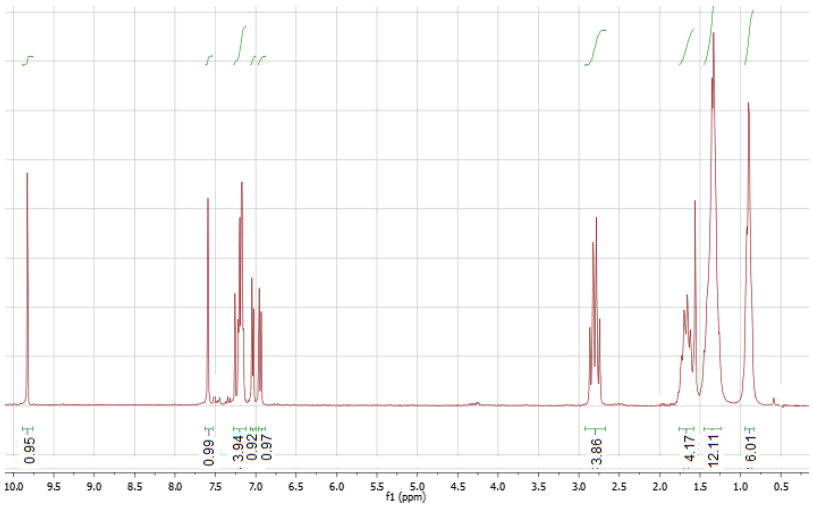
Journal: New Journal of Chemistry



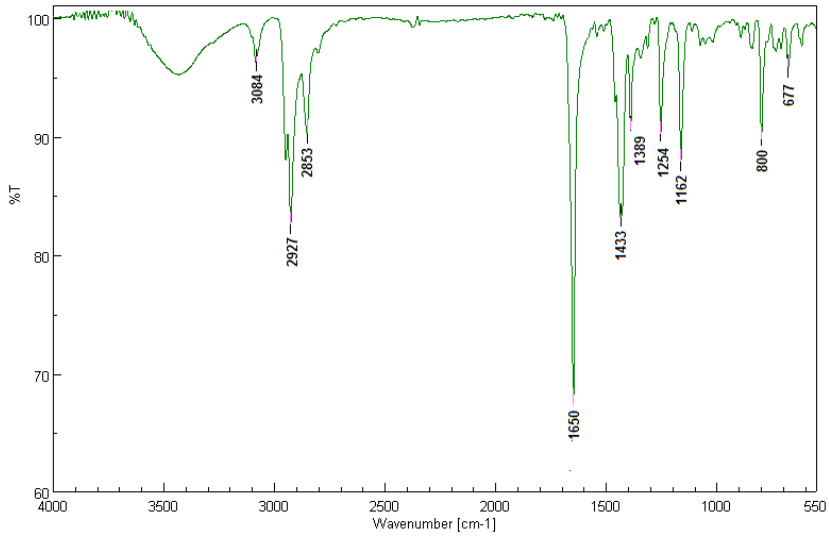
^{1}H-NMR ($CDCl_3$) Spectrum of (1,4-phenylenebis(methylene))bis(triphenylphosphonium) bromide (phosphonium sal). ^{1}H-NMR ($CDCl_3$, δ): 7.60 m(30 H phenyl aromatic), 6.91 s (4H, aromatic), 5,40 s(2H aliphatic), 5,34 s(2H aliphatic).



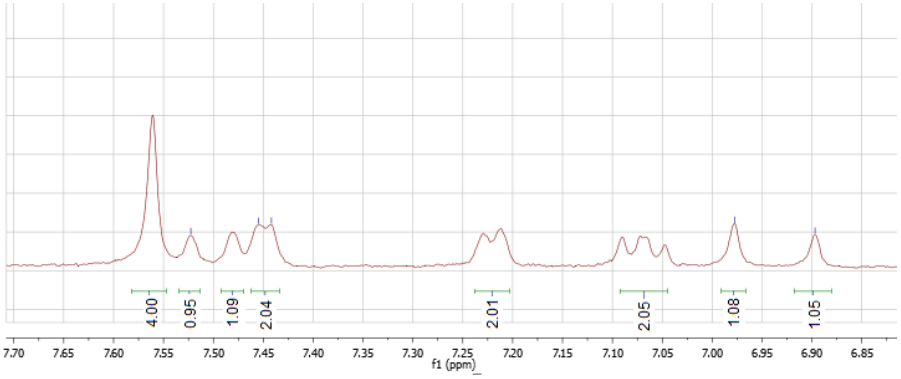
FT-IR spectrum of (1,4-phenylenebis(methylene))bis(triphenylphosphonium) bromide (phosphonium sal). FT-IR (KBr): vCH at 3046 cm^{-1} and 3005 cm^{-1} (aromatic), vCH at 2876 cm^{-1} and 2776 cm^{-1} (aliphatic groups), vC=C at 1618 cm^{-1}, 1584 cm^{-1} (aromatic rings), γCH (para-disubstitution pattern) at 837 cm^{-1}.



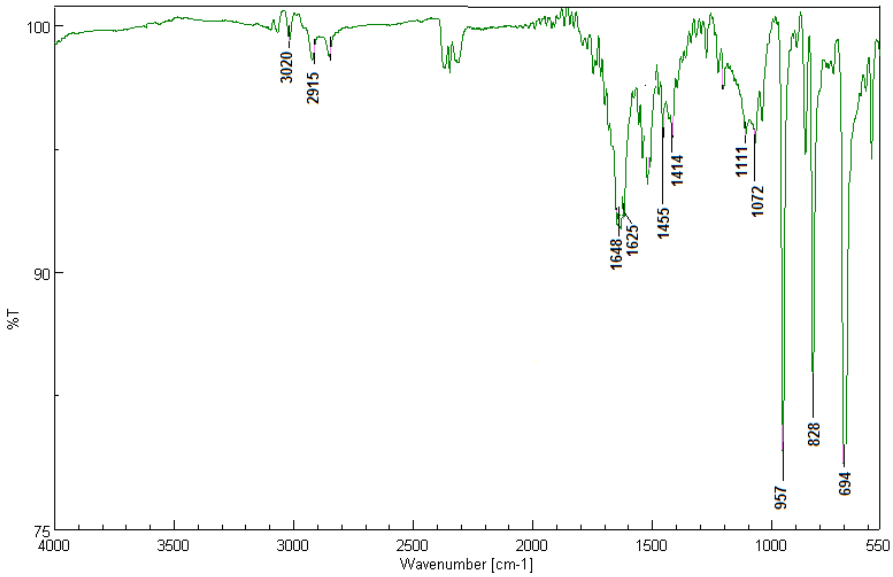
^{1}H-NMR ($CDCl_3$) Spectrum of 3,3'''-dihexyl-[2,2':5',2'':5'',2'''-quaterthiophene]-5-carboxaldehyde 9.83 s(1H, -CHO), 7.59 s (1H aromatic), 7.26-7.15 m(4H, aromatic), 7.03 d(1H aromatic), 6.94 d (1H aromatic), 2.81 dd(4H, Th-CH_2-), 1.66 dd(4H, -CH_2-), 1.33 m(broad, 12H, -CH_2-CH_2-CH_2-), 0.88 m(broad, 6H, -CH_3).



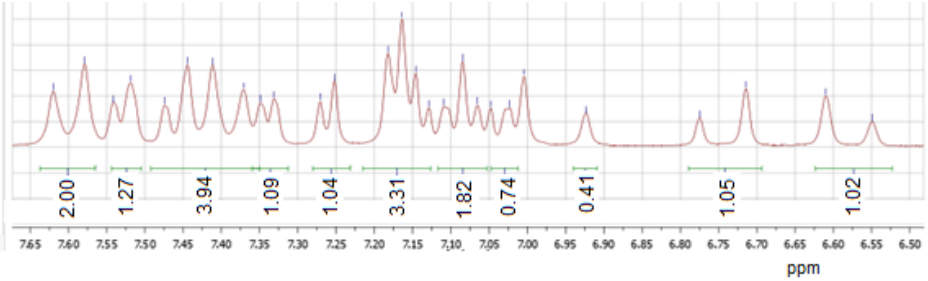
FT-IR spectrum of 3,3'''-dihexyl-[2,2':5',2'':5'',2'''-quaterthiophene]-5-carboxaldehyde (KBr, cm^{-1}): νCH at 2949, 2927 and 2853 (aliphatic groups), νC=O at 1650 (carbonyl group), νC=C at 1433, (aromatic rings).



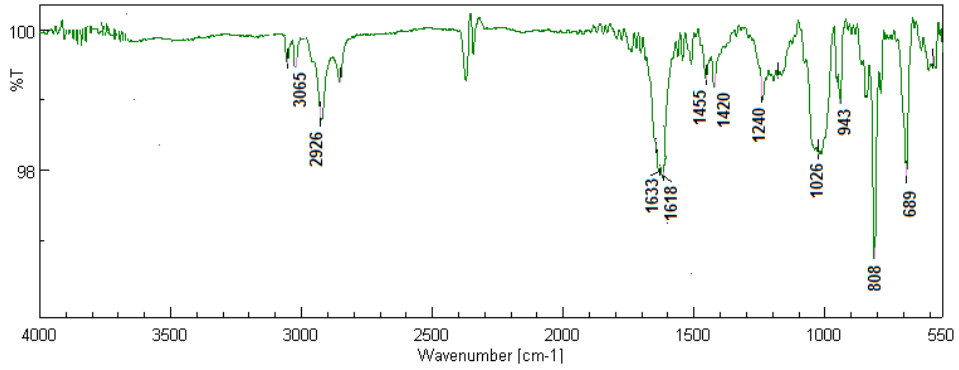
^{1}H-NMR (DMSO-d_6) spectrum of 1,4-bis(2-(thiophen-2-yl)vinyl)benzene, labeled as FV1Th: 7.56 s(4H, phenylene group), 7.52 and 7.44 (d, 16 cps, 2H vinylene), 6.98 and 6.89 (d, 16 cps, 2H vinylene), 7.45 d(2H Th), 7.23 d (2H Th), 7.07 dd(2H, Th).



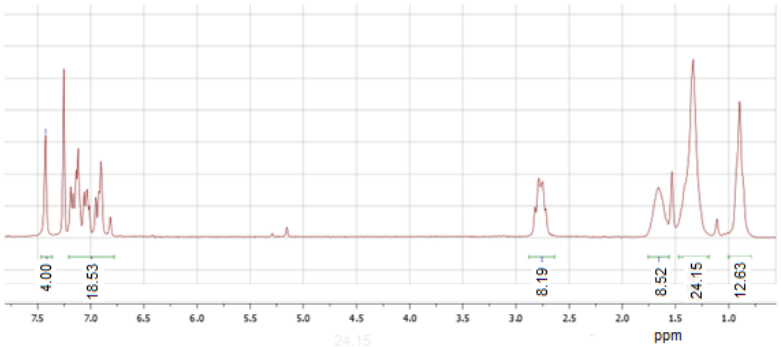
FT-IR spectrum of 1,4-bis(2-(thiophen-2-yl)vinyl)benzene, labeled as FV1Th, FT-IR (KBr): νCH at 3020 cm^{-1}, νC=C at 1625 cm^{-1} and 1518 cm^{-1}; νC=C at 957 cm^{-1} (vinylene group), γCH (p-disubstitution pattern benzene ring) at 828 cm^{-1}; γCH (thiophene ring) at 694cm^{-1}.



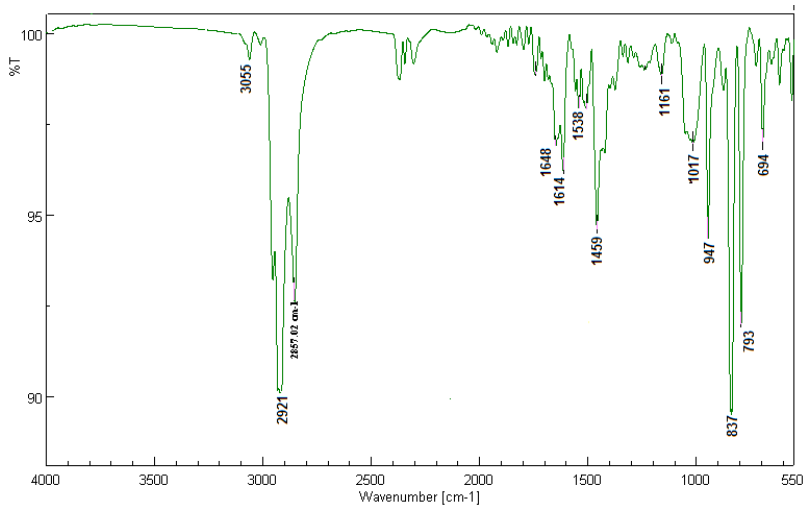
^{1}H-NMR (DMSO-d6, δ) spectrum of (1,4-bis(2-([2,2'-bithiophen]-5-yl)vinyl)benzene), labeled as FVBiTh. 7.60 d(2H), 7.53(d, 1H), 7.43 (dd, 4H phenylene group), 7.34 (d, 1H), 7.26 (d, 1H), 7.15 (m, 3H), 7.09 (t, 2H), 7.04 (d, 1H), 6.96 (d, 1H, vinylene), 6.74 (d, 1 H vinylene), 6.58 (d, 1H vinylene).



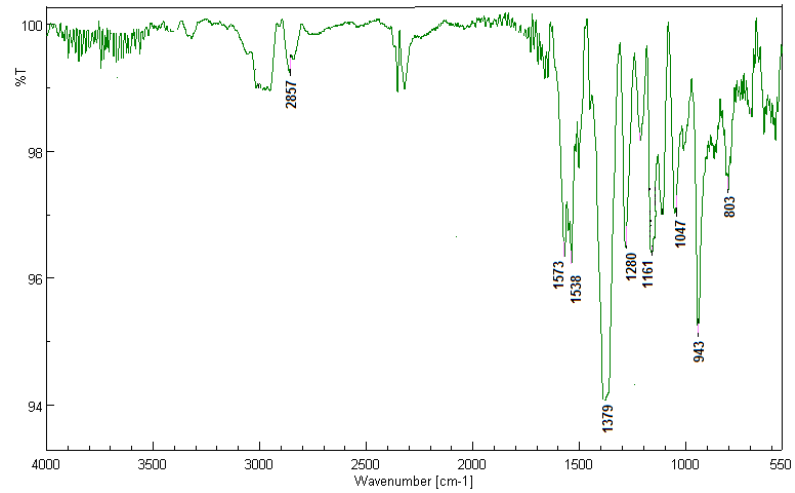
FT-IR spectrum of (1,4-bis(2-([2,2'-bithiophen]-5-yl)vinyl)benzene), labeled as FVBiTh: νCH at 3065 cm^{-1}, νC=C at 1633 cm^{-1} and 1618 cm^{-1}; νC=C at 943 cm^{-1} (vinylene group), γCH (p-disubstitution pattern benzene ring) at 808cm^{-1}; γCH (thiophene ring) at 689cm^{-1}.



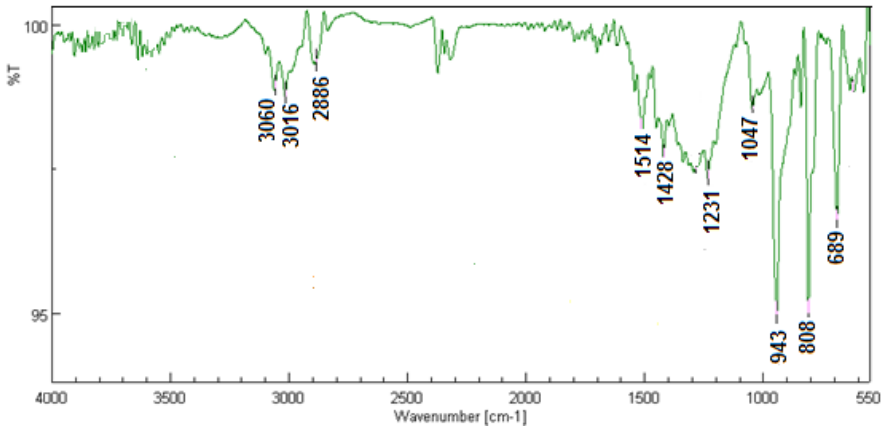
^{1}H-NMR ($CDCl_3$) spectrum (1,4-bis(2-(3,3'''-dihexyl-[2,2':5',2'':5'',2'''-quaterthiophen]-5-yl)vinyl) benzene), labeled as FVTeTh. ^{1}H-NMR ($CDCl_3$), δ): 7.43 s(4H aromatic), 7.18-6.80 m(18H aromatic), 2.75 dd(8H aliphatic, Th-CH_2-), 1.66 s (broad, 8H aliphatic –CH_2-), 1.33 s (broad, 24H aliphatic –CH_2-CH_2-CH_2-), 0.90 s (broad, 12H aliphatic, -CH_3).



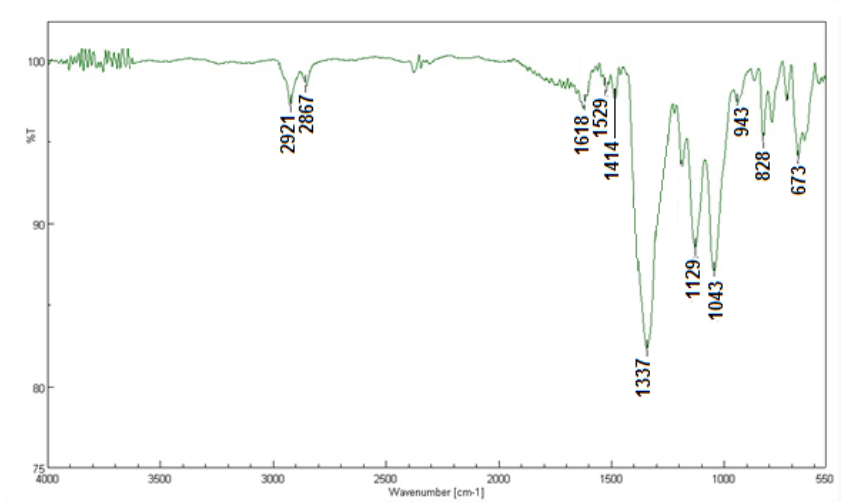
FT-IR spectrum of (1,4-bis(2-(3,3'''-dihexyl-[2,2':5',2'':5'',2'''-quaterthiophen]-5-yl)vinyl)benzene), labeled as FVTeTh.



FT-IR (KBr) spectrum of poly(FV1Th): νCH at 3005 cm^{-1} (aromatic ring), νC=C at 1573 cm^{-1} and 1538 cm^{-1}, νC=C at 943 cm^{-1} (vinylene group), γCH (p-disubstitution pattern benzene ring) at 803 cm^{-1}; γCH (thiophene ring) at 699 cm^{-1}.



FT-IR (KBr) spectrum of poly(FVBiTh): νCH at 3016 cm^{-1} (aromatic ring), νC=C at 1514 cm^{-1}, νC=C at 943 cm^{-1} (vinylene group), γCH (p-disubstitution pattern benzene ring) at 808 cm^{-1}; γCH (thiophene ring) at 689 cm^{-1}.



FT-IR (KBr) spectrum of poly(FVTeTh): νCH at 2921 cm^{-1} and 2867 cm^{-1}(aliphatic groups), νC=C at 1618 cm^{-1}, 1529 cm^{-1} (aromatic rings), νCH at 943 cm^{-1} (vinylene group), γCH (p-disubstitution pattern benzene ring) at 828 cm^{-1}; γCH (thiophene ring) at 673 cm^{-1}.