Supporting Information

Absorption and Fluorescence Spectra of Poly-(p-phenylene vinylene) (PPV) oligomers: An Ab Initio Simulation

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Table S1– Stilbene geometry parameters calculated at the RI-MP2/SV(P) level. Frozen core corresponds to calculations done with the first 14 orbitals frozen, and frozen (core+14), to the first 28 orbitals frozen. Atom labels are identified in Scheme S1.

	Frozen core	Frozen (core +14)
Bond distances (Å)		
C2-C3	1.356	1.358
C3-C4	1.466	1.482
C4-C5	1.408	1.409
C5-C6	1.397	1.400
C6-C7	1.400	1.402
C7-C8	1.401	1.403
C8-C9	1.397	1.399
C9-C4	1.409	1.411
C2-H1	1.100	1.079
C5-H3	1.097	1.071
Angles (degrees)		
H1-C2-C3	118.72	119.20
C2-C3-C4	125.32	124.45
C3-C4-C5	119.39	119.33
C4-C5-C6	121.04	120.64
Dihedral Angles (degrees)		
C1-C2-C3-C4	180.62	181.20
C2-C3-C4-C5	24.82	24.29
H1-C2-C3-C4	3.40	3.27
H2-C3-C4-C5	22.11	22.24
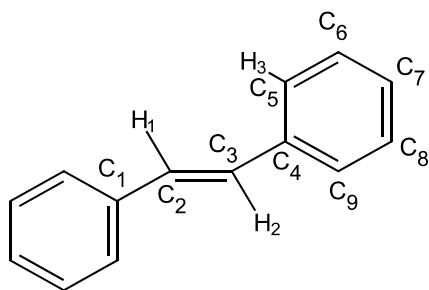
Scheme S1 – Atom-labeling scheme for stilbene.