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# Tuning of optical properties of *p*-phenyl ethenyl-*E*-furans: A Solvatochromism and Density functional theory

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## Abstract

*p*-Phenyl ethenyl-*E*-furans (**1-6**) with varied electron donor and acceptor substituent ($NO_2$, CN, Cl, H, $OCH_3$, $NH_2$) were synthesized and studied the substituent induced optical properties (dipole moment, transition dipole moment, oscillator strength, optical band gap, hyperpolarizability) using Solvatochromism and Density functional theory. It is shown that furan acts as a weak electron donor in presence of an electron withdrawing *p*-phenyl substituent ($NO_2$, CN, Cl), whereas furan acts as a weak electron acceptor in presence of an electron donating *p*-phenyl substituent ($OCH_3$, $NH_2$). In comparison to ethenylfuran **4**, the HOMO-LUMO energy band gap is decreased upon increasing the electron donating or electron withdrawing nature of the phenyl ring. Calculation of excited state dipole moment and polarizability of **1-6** in solvent of varying polarity suggest that the nitro and amino compounds (**1, 6**) exhibit charge transfer excited state, whereas excited state of compounds **3-5** is non-polar in nature. As compared to the ethenylfuran **(4)**, the first hyperpolarizability (β) is increased in presence of a strong electron withdrawing or strong electron donating *p*-phenyl substituent**.** The higher $\beta$ value is found for