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Length-Dependence of Electron Transfer in Conjugated Molecular Wires SHASHI KARNA, GOVIND MALLICK, US Army Research Laboratory, RAVINDRA PANDEY, Michigan Tech University — The electron transfer (ET) properties of π-electron conjugated molecular wires consisting of polyene chain, $[>\mathrm{C}=\mathrm{C}<]_{n,(n=1-11)}$ has been investigated in the framework of *ab initio* molecular orbital theory. As expected, magnitude of the ET coupling matrix element V_{DA} decreases exponentially with increase in the length of the molecular wire. However, in contrast with the rigid σ-bonded molecular wires, the decay constant, β, for the conjugated systems exhibits three different regimes over the calculated length. This is attributed to the delocalized nature of the electrons along molecular length that facilitates retention of the electron coupling even at large separations between the donor and acceptor centers.

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