Dipole moments of polyenic oligomeric systems. Part I. A One-dimensional molecular wire model

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Ground-state dipolar moments of oligomeric compounds, containing electron-donor (D) and electron-acceptor (A) groups as two terminal units of the polyenic bridge (D-wire-A), can well be described by means of a one-dimensional molecular wire model, which considers a scattering process of electrons through the charge-transfer conduction channel. The dipole moment of the oligomers (?n) follows a non-linear dependence of the polyenic bridge length (L) according to ?n = ?0 + ?? (1 - e-?L) where ?0 is the dipole moment of the first compound of the series, without a polyenic unit (n = 0), ?? is a limit value for L ? » ? and ? is the one-dimensional conduction constant of the ?-molecular orbital channel of the molecular wire. This model can be extended to all those conjugated oligomers of the D-wire-A type where the electronic charge of the donor group can induce a soliton wave as far as through the polyenic bridge towards the acceptor group.