Bridge effect in charge-transfer photoconductiom channels. 1. Aromatic carbonyl compounds

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During the charge-transfer process in the excited state of aromatic carbonyl compounds, the local C-O net charge decreases as the polyene bridge length between the aromatic and the carbonyl systems is increased. Part of the photoinduced electronic charge, transferred through this molecular wire from the aromatic ring to the carbonyl acceptor group, is retained by the ?-conduction channel of the polyene molecular wire ("bridge effect"). The present study defines the quantum molecular resistance in these polyene photoconduction channels by means of an analysis of the molecular excited states for isolated systems, based on semiempirical molecular orbital calculations (MNDO, CNDO/S). © 1993 American Chemical Society.