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Structural and spectroscopic properties of a set of donor-acceptor molecules with and without spacers**Part 1. Methoxyphenyl and dimethylaminophenyl groups as donors**Nessima Salhi¹, Leif A. Eriksson, Jean-Louis Calais[✉] and David Nordfors²

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Abstract

Four D π A systems (Donor- π -link-acceptor) have been investigated by means of semiempirical and ab initio procedures. The geometries of the ground states have been optimized with the MNDO and AM1 methods, with consistent results. Very small energy differences were found in ab initio Hartree-Fock calculations on the semiempirically optimized planar and unconstrained structures. Charge distributions and dipole moments have been calculated. The INDO-CI program zindo has been used to calculate transition energies and oscillator strengths for excitations from the ground states. It is found that for the molecules with an insulating spacer group, the main transitions are local excitations within the donor or acceptor groups. When no spacer is present the HOMOs and LUMOs are more delocalized, leading to very small charge transfer effects upon excitation.

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