

Abstract Submitted
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The influence of donor-acceptor groups on the excited-state dynamics of ethylenic molecules¹ ANJA ROEDER, Department of Chemistry, University of Ottawa, Canada, ANDERS SKOV, Department of Chemistry, University of Copenhagen, Denmark, ANDREY E. BOGUSLAVSKIY, KATHERINE HERPBERGER, RYAN J. MACDONELL, MICHAEL S. SCHUURMAN, ALBERT STOLOW, Department of Chemistry, University of Ottawa, Canada — Conical intersections (CIs) govern molecular dynamics in many light-driven processes, such as vision or photophysics. The non-adiabatic dynamics of ethylene, the simplest double-bond containing molecule, has been extensively investigated as a model system: after initial excitation to the * state, the molecule deforms on its way to the CI - it simultaneously twists along the C=C bond and pyramidalizes on one of the carbons, before returning to a vibrationally hot ground state. The pyramidalization is also associated with an increase in electron density: can we, by changing the electron density on either side of the double bond a priori of the dynamics, control and tune the photophysics of ethylene? To answer this question, we explored the excited-state dynamics of a series of donor-acceptor substituted ethylenes, namely acrylonitrile (acceptor-substituted), methylvinylether (donor-substituted) and 3-methoxyacrylonitrile (donor and acceptor substituted). This joint time-resolved photoelectron spectroscopy and ab initio molecular simulation investigation demonstrates both experimentally and theoretically the fascinating involvement of the donor-acceptor groups in the excited-state dynamics of the double bond.

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