

PULSE INDUCED DARK STATE OF ACETYLENE

ANTOINE AERTS, *SQUARES, Université Libre de Bruxelles, Brussels, Belgium*; PASCAL KOCKAERT, SIMON PIERRE GORZA, *OPERA Photonique, Université libre de Bruxelles, Brussels, Belgium*; JEAN VANDER AUWERA, NATHALIE VAECK, *SQUARES, Université Libre de Bruxelles, Brussels, Belgium*.

We simulate laser-induced dynamics in acetylene (C_2H_2) using fully-experimental structural parameters. The rotation-vibration energy structure, including anharmonicities, is defined by the global spectroscopic Hamiltonian for the ground electronic state of C_2H_2 built from the extensive high resolution spectroscopy studies on the molecule, transition dipole moments from intensities, and effects of the (inelastic) collisions are parametrized from line broadenings using the relaxation matrix [J. Chem. Phys. **154**, 144308 (2021)]. The approach, based on an effective Hamiltonian outperforms today's *ab initio* computations both in terms of accuracy and computational cost, however, is limited to a few small molecules. With such accuracy, the Hamiltonian permits to study the inside machinery of theoretical pulse shaping [J. Chem. Phys. **156**, 084302 (2022)] for laser quantum control. With an adequate pulse shaping technique (in mid-IR) based on “super-Gaussian” pulses, we show a realistic and performant path to the population of a “dark” ro-vibrational state in C_2H_2 .