

I. MOTIVATION

The existence of nuclear-spin isomers was reported for the first time in 1927 by Heisenberg and Hund to explain anomalous properties of molecular hydrogen [1, 2]. However, the experimental separation and/or conversion of nuclear spin isomers of polyatomic molecules is a very challenging problem. In the last years, several theoretical models [3–8] have been proposed showing different behavior of the nuclear spin isomers after light excitation.

In contrast to systems such as hydrogen or water, where the exchange of the two hydrogens is related to an overall rotation of the molecule, in these theoretical proposals the molecules possess an internal torsional degree of freedom that exchanges the two hydrogen atoms, and thus relates the different classes of nuclear spin isomers [9]. Using model systems of reduced dimensionality, these previous works have shown that the differences on the excited state dynamics are due to the quantum interferences of the initial nuclear wave function built up for each nuclear spin isomer.

II. WORK PLAN

Previously, we have worked on the excited state dynamics of the nuclear spin isomers of 1,1-difluoroethylene (DFE) using exact quantum dynamics in the torsional degree of freedom [8]. We were able to distinguish between the nuclear spin isomers of DFE through the interference on the excited state. Now, we would like to study the effect of switching on all the degrees of freedom to check whether these interference effects still remain. For this purpose, the method of choice is the multi-configurational time-dependent Hartree (MCTDH), as it can treat systems up to about 1000 degrees of freedom including quantum effects [11]. Previously, we have calculated potential energy surfaces and couplings with *cc-pvdz/SA(11)-MS-CASPT2(2,6)* in the CH_2 pyramidalization, CF_2 pyramidalization, torsion and C-C stretching normal modes. The remaining normal modes (8) will be approximated as harmonic oscillators. These adiabatic potentials will be transformed to a suitable basis to be used by MCTDH [10]. The initial conditions were already calculated and implemented in MCTDH. It is still under discussion in which terms we will express the kinetic energy operator. Hopefully, by the end of the stay, the dynamics will have shown us some differences in the excited state behaviour of these nuclear spin isomers.

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