Supplementary Information

for

Wavepacket Dynamics of the Axially Chiral Molecule Cl-O-O-Cl under Coherent Radiative Excitation and Including Electroweak Parity Violation

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The present supplementary material as described in the appendix of the full paper contains the program package used for the computations (see also Fig. 27 for an overview).

This is a documentation for the latest working version of RPH using sin/cos-fitting and analytical derivatives. Torsional levels and tunneling splittings of Cl-O-O-Cl are calculated for the hypothetical symmetric potential. All programs were compiled using a commercially available Intel Fortran 90 compiler (ifort, v.11.1. For use with other compilers adjust accordingly). The numerical precision is set to double precision (128 bit, corresponding to a real floating point number with 32 decimal digits). Copy cloocl.zmat, the folder data, including the ab-initio outputs, *.f and *.f90 source codes and execution files (*.cm) into the same folder or adjust accordingly. The file rph.chk is a sample output for a calculation with 199 gridpoints that reproduces the numbers given in the paper.

How to execute

The program consists of several subprograms which are to be executed in the following order:

1. Execute compile_sub.cm. This creates objects (.o and .mod-files) used for further compilation.

2. Execute mkinrph.cm. This converts the input from Quantum Chemical calculations (Gaussian .log.out-files to be found in the folder data) and the Z-matrix definitions (cl2o2.zmat) to the specific RPH format.

3. Execute rph_fit.cm. This fits the numerical data to a cos/sin-series expansion.

4. Execute rph_ham.cm. This prepares the Hamiltonian by calculating the effective potentials, metric g-tensor elements and B-matrix elements (Coriolis type couplings).

5. Execute rph.cm. This sets up the Hamiltonian matrix and solves it on an equidistant grid using standard DVR.

For details of the theory consult section 2 of the paper and references given therein.

List of all files

Name:	Description
cloocl.zmat	Z-matrix file
*.log.out	ab initio outputs (in data folder)
structs.f90	
markfit.f90	
diabat.for	
sub.f90	
compile_sub.cm	compiles above objects for further use throughout the following routines.
mkinrph.f	program code to read and format ab initio output
mkinrph.cm	runs compilation and execution of mkinrph
rph_fit.f90	program code to fit ab initio outputs to sin/cos-series expansion.
rph_fit.cm	runs compilation execution of rph_fit
rph_ham.f90	program code to calculate potentials and corrections along the reaction path
rph_ham.cm	runs compilation and execution of rph_ham
rph.f90	program code to calculate eigenfunctions and eigenenergies
rph.cm	runs compilation and execution of rph
rph.chk	sample output for 199 gridpoints