The parameters Es and Eeff determine the energy split of the excited vibrational states. Therefore, the results should be **averaged over the rovibrational wavefunction.**

It was claimed in [Prasannaa et al.(2019)] that these parameters are sensitive to the bending of the molecules and, thus, the **averaged result should differ significantly** from the equilibrium value.

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RaOH

$\mathcal{P},\mathcal{T}$-odd parameters for the RaOH molecule.

	E_{eff}, $\frac{\text{GV}}{\text{cm}}$	E_s, (kHz)
Equilibrium	−48.866	−64.788
$v = 0$	−48.863	−64.784
$v = 1$	−48.585	−64.416
cGHF RaOH [Gaul, Berger (2020)][a]	−56.2	−75.6
cGKS RaOH [Gaul, Berger (2020)][b]	−49.3	−66.4

[a] $\Omega = 0.494$.
[b] $\Omega = 0.471$.

YbOH

Sensitivities to the $\mathcal{P},\mathcal{T}$-odd effects for YbOH

	E_{eff}, GV/cm	E_s, kHz
Equilibrium geometry	23.875	20.659
$v = 0$ state	23.810	20.602
$v = 1$ state	23.740	20.540
FSCC+Gaunt [Denis et al.(2019)]	23.37	
QZ CCSD [Prasannaa et al.(2020)]	23.80	
cGHF [Gaul, Berger (2020)]	23.57	20.60
cGKS[a] [Gaul, Berger (2020)]	17.48	15.25

[a] For the value of $\Omega = 0.495$.

The potential surface (**CCSD(T)**) and electronic structure (**CCSD**) of the RaOH and the YbOH molecules are computed taking into account relativistic effects and spin-orbit interaction
Heavy atoms are modeled using GRECP developed in PNPI

We show that the PT-odd parameters do not have significant sensitivity to the vibrations

The spectrum of the vibrational wavefunctions allow us to compute l-doubling

The value of l-doubling is calculated:

RaOH: ΔE=14 MHz ***DOI: 10.1103/PhysRevA.103.032819***

YbOH: ΔE=26 MHz ***coming soon***

The developed technique will later be used for calculations in the external fields