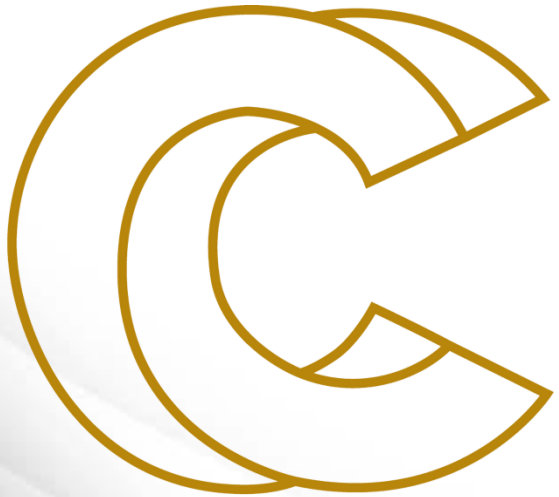

EURO^2

Electronic structure calculations by Gaussian 16

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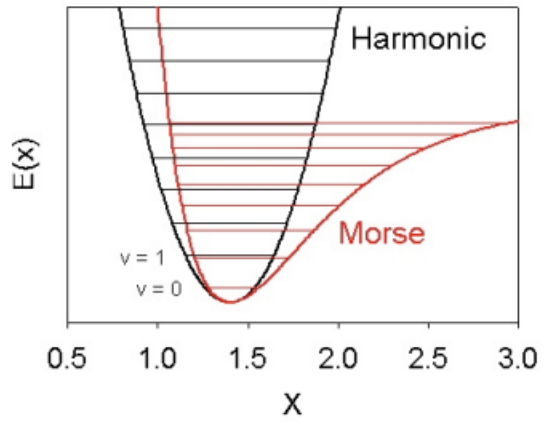
By using Freq Command

- Frequency calculations in Gaussian, this is calculated by default using freq command, calculates force constants and the resulting vibrational frequencies.
- VCD, ROA, Raman calculations can be extracted. https://gaussian.com/freq/
- First-order approximation (even harmonic) is used, so only fundamental bands with a non-zero intensity are allowed.
- Correction of frequencies with a scaling factor (DFT ~ 0.98)

https://cccbdb.nist.gov/vibscalejustx.asp

$$\text{IR Intensity} \propto \left(\frac{\partial \mu}{\partial q}\right)^2 \propto \left(\frac{\partial^2 E}{\partial R \partial F}\right)^2$$

- μ - Dipole Moment
- q - Normal Coordinates
- E - Energy
- R - Nuclear Coordinates
- F - External Electric Field

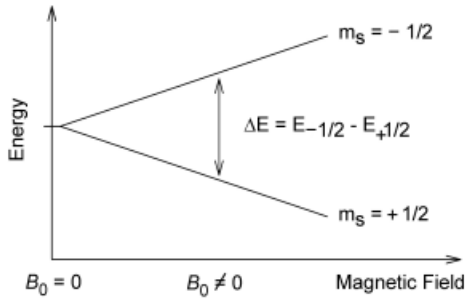


NMR spectrum

NMR command

- It is necessary to calculate the NMR standard molecule (i.e. TMS-Trimethylsilane) at the same level of theory as the molecule of interest.

$$\text{NMR Shielding} \propto \left(\frac{\partial^2 E}{\partial B \partial I}\right)$$



- E - Energy
- B - External Magnetic Field
- I - Nuclear Magnetic Moment (Nuclear Spin)

$$\text{Spin} - \text{Spin Coupling} \propto \left(\frac{\partial^2 E}{\partial^2 I}\right)$$

In Gaussian16: Continous Set of Gauge Transformations (CGST) and the Gauge Independent Atomic orbitals (GIAO) methods are available.

NMR spectrum

GIAO is a default method.

NMR shielding tensors and magnetic susceptibilities using the Hartree-Fock method, all DFT methods and the MP2 method

CSGT calculations require large basis sets to achieve accurate results.

Magnetic susceptibilities may also be computed with both GIAOs and CGST.

Spin-spin coupling constants may also be computed during an NMR job.

The chemical shift δ is obtained from σ by

$$\delta = \sigma_{ref} - \sigma,$$

Example command: NMR=(GIAO,spinspin,mixed)
SpinSpin: Compute spin-spin coupling constants

Thanks

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