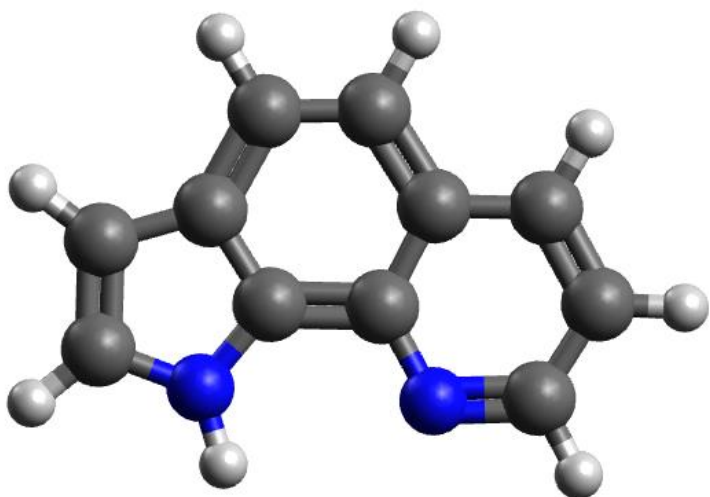


# 1H-Pyrrolo[3,2-h]quinoline



## Benchmark for Vibrational Frequencies:

*J Phys Chem A* **116**: 11973 (2012)

doi:10.1021/jp309618b

$C_s$  Point Group → *No Degenerate Modes*

21 Atoms → 57 Modes → *Robust Statistics*

Rigid Molecule → *No Large-Amplitude Motions*

## Geometry and Frequencies with ORCA v3.0.3

! PBE def2-TZVP def2-TZVP/J RI TIGHTOPT GRID4 VERYTIGHTSCF

## Unweighted Normal Modes

$$\vec{L}^X = \begin{bmatrix} | & | & & | \\ \vec{\ell}_1^X & \vec{\ell}_2^X & \dots & \vec{\ell}_n^X \\ | & | & & | \end{bmatrix}$$

$$X = \begin{cases} \Delta = [10^{-4}, 10^{-1}] \text{ Bohr} \\ \text{or} \\ \text{"A"} \text{ (analytical)} \end{cases}$$

"Best  $\Delta$ " → Minimize MAD[ $\Delta$ ]

$$\text{MAD}[\Delta] \equiv \frac{1}{n} \sum_i \left| 1 - \left| \vec{\ell}_i^A \cdot \vec{\ell}_i^\Delta \right| \right|$$

## MAD & MaxAD of Frequencies

$$\text{MAD}[\tilde{\nu}^\Delta] = \frac{1}{n} \sum_i |\tilde{\nu}_i^A - \tilde{\nu}_i^\Delta|$$

$$\text{MaxAD}[\tilde{\nu}^\Delta] = \max\{|\tilde{\nu}_i^A - \tilde{\nu}_i^\Delta|\}$$

